# Data & Analysis Preservation: status update

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#### This presentation

- An introduction to the PHENIX website redesign was presented in March 2020:
  - https://docs.google.com/presentation/d/1Vng0wl9PyZKYmfRw\_k9ZOHko6lwZDDQymUixDA-Srvg/edit?usp=sharing
  - Please see the link above for a more generic discussion of motivations, technology choices etc
- Discussion today: current status of the website
  - Leveraging the available cloud resources
  - How to ensure usefulness of the website as a component of Analysis Preservation and its potential to advance more immediate goals of PHENIX
- Evaluating containers for analysis preservation, training and general improvement of software deliver and use in PHENIX
- Leveraging the website and other tools for the PHENIX School



#### The website: a bit of history

- The legacy PHENIX website had been showing its age for a while
  - Some useful information was spread over multiple web servers
  - Used as a document repository with limited functionality and lack of external visibility
  - Certain software modules (PHP) in its framework were potentially vulnerable security-wise
- Technical problems encountered in 2020 illustrate operational risks due to difficulty of upgrades e.g. maintaining the legacy software stack in the evolving OS environment while staying abreast of security requirements
- Less DB support available as time goes on (actually none at this point)



### Strategy 2020

- DAP = Data and Analysis Preservation
- Design a new website aligned with the goals of DAP
  - Emphasis on ease of maintenance and long-term durability
  - Collect and curate materias from available resources
  - Create new materials where necessary
- Factor out the repository and other similar functionality by leveraging modern solutions developed and employed in the NP and HEP communities
  - The website effectively becomes a portal to cloud resources, with a moderate amount of material still hosted locally

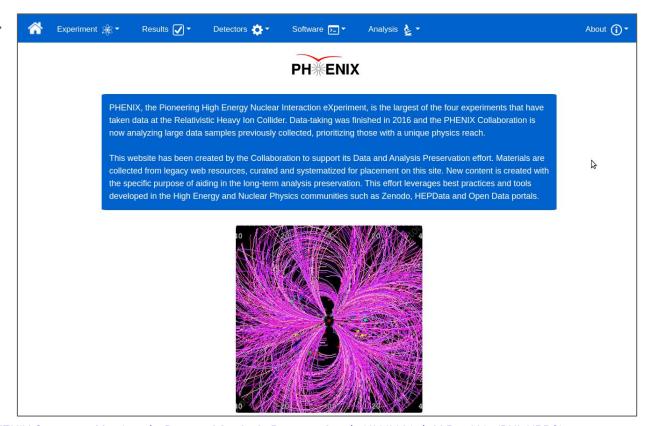
### The website technology and status

- Use a static website generator for speed and security
- Content and layout are separate; easy to use markup (not HTML)
- Data kept in specially formatted files (YAML) to provide DB-like functionality without having an actual database
  - Flexibility and consistency across multiple pages define data once, use in many places
  - Powerful macros can be created
- All materials hosted transparently on GitHub
  - Leveraging free hosting of the development version of the website on GitHub pages
- As of Fall 2020 the production version is hosted at BNL at the canonical URL: <a href="https://www.phenix.bnl.gov/">https://www.phenix.bnl.gov/</a>
  - Releases approximately every two weeks
- In the following few slides we will review the site

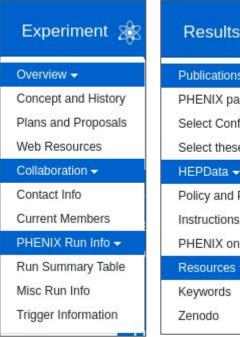


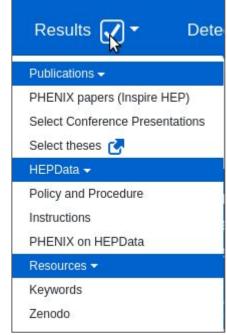
#### Website: the landing page

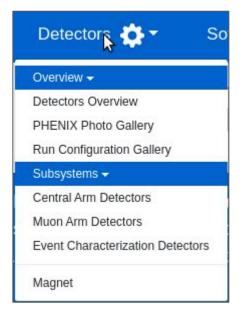




# Website: dropdown menus (1)







### Website: dropdown menus (2)







#### Leveraging the community cloud resources

- Use well established solutions widely adopted in the community
  - NB. solid back-end and support
  - Look at best practices at CERN and other labs
  - Reduces cost and increases long-term viability of the PHENIX Web infrastructure
- Resources already adopted by PHENIX
  - Zenodo (a general-purpose digital repository)
  - HEPData a repository for numerical data used in publications
  - InspireHEP a searchable publication catalog
- So a few types of functionality effectively migrated to the cloud from the legacy site
- Heavy investment in Zenodo and HEPData
- Upcoming
  - OpenData: a DAP-oriented portal for sharing datasets, software and documentation
  - REANA: a framework for reproducible analysis based on containerization



#### CERN and community tools for DAP



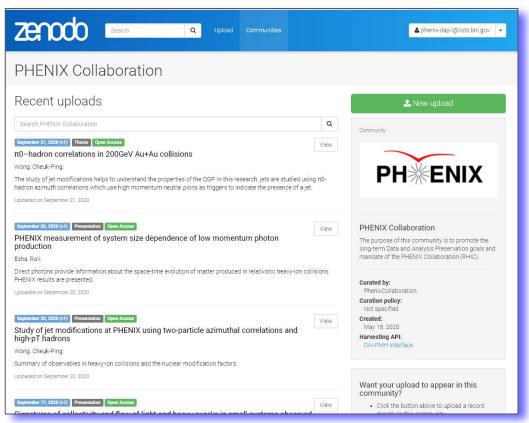
#### Zenodo

- Zenodo close to 200 PHENIX items were made available on the portal
- DOIs are an important feature for long-term preservation ("permalink")
- Uploaded and tagged ⅔ of PHENIX theses with keywords (currently at 124), work in progress with completion date in 2021 - thanks to Stacyann Nelson
- Steady upload of conference/workshop and other presentation, with a dedicated page on the new site
- Keywords essential for discoverability and integrity of references
  - A list is curated, updated and used with all uploads

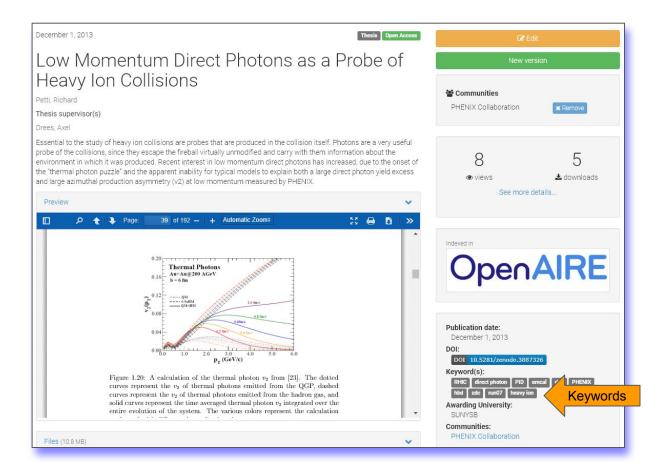


# Zenodo@CERN - the PHENIX community

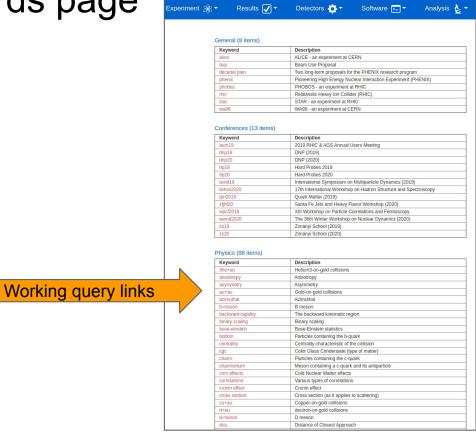
- Branded
- Curated
- Discoverable
- Indexed (keywords)
- Elastic search capability



# An example of a PHENIX item on Zenodo



### Zenodo keywords page





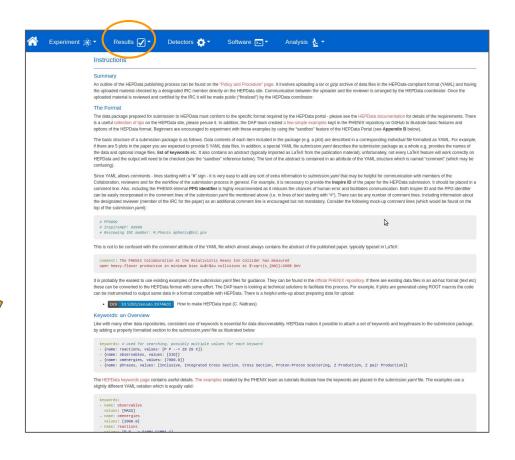
#### **HEPData**

- A repository for numerical data used in publications (e.g. data points in plots).
- Standard practice in many experiments.
- We are still catching up with other major experiments who started investing in this earlier.
- Data from 46 published PHENIX papers has been uploaded
  - Available for reliable download in a standard format
  - Indexed and discoverable.
  - Once again, DOIs.
- The official publication policy in PHENIX mandates the HEPData process for each potential publication. Steady state work now.
- HEPData/Rivet workshops in Fall 2020 (thanks to Christine for organizing this).
- Based on our experience the policies and procedures have been discussed and updated.
  - Extensive re-write of the corresponding documentation on the website (next page)



# HEPData Instructions and Policies

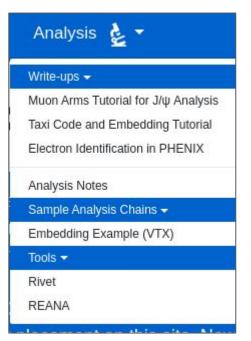






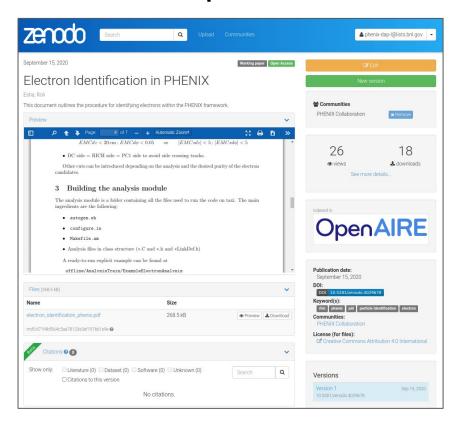
### Analysis resources on the site

- Progress has been made with creating updated tutorials for specific work areas (see on the site)
- Currently implemented as write-ups published on Zenodo and linked on the site
- Caveat: these materials need another round of updates to account for mode code access (i.e. update or eliminate references to the code browser only available internally, review placement of code on AFS and whether it's suitable for publication etc)





#### Example of a tutorial uploaded to Zenodo



### The analysis content

- Having well documented use cases (tutorials and/or complete preserved analyses) is obviously conducive to both efficiencies in medium term and longer term DAP
- Better engagement by the PHENIX community still remains on the critical path
  - Reverse engineering of prior analyses turns out to be close to impossible
  - Analyzers active in a given area are the best resource we have to create materials to meet education and analysis preservation goals
- We have good technology when it comes to all aspects of DAP implementation (Zenodo, REANA etc)
  - Can upload and systematize complete datasets, software, all sorts of documentation
- ...but the actual materials still need to be produced

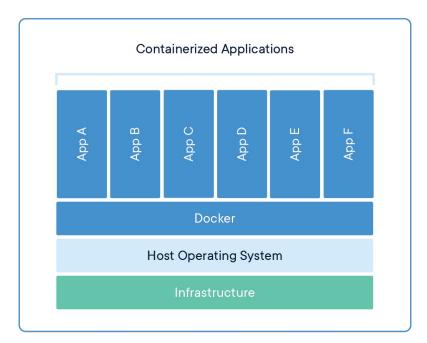


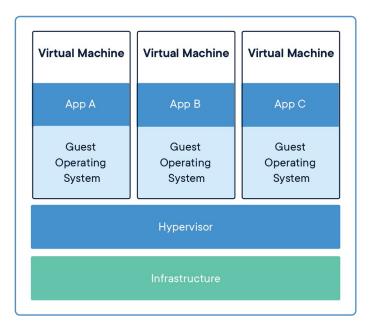
#### Containers

- Containerization is a methodology of packaging software into standardized units for development, shipment and deployment. There are two leading platforms:
  - Docker concept and implementation coming from industry
  - Singularity originated at LBNL, contributions from Fermilab, adopted in the Open Science
     Grid and many other venues for scientific computing used for PHENIX production
  - A high degree of interoperability between the two
- In the following slides some basic Docker concepts will be introduced, apologies to those of you already familiar with the technology
  - There is a plethora of information on the Web for your perusal
  - https://docs.docker.com/
- Both Containers and Virtual Machines provide a layer of abstraction on top of the host operating system thus making deployment possible in a variety of environments
  - But they do it differently



#### Containers vs VM





- Virtual machines require a "hypervisor" which is responsible for complete emulation of an OS
- However containers share the same OS kernel resulting in more economical storage and better performance
- Containers are made possible by the Linux resources isolation features
   PHENIX Conveners Meeting ◆ Data and Analysis Preservation ◆ 1/20/2021 ◆ M.Potekhin (BNL NPPS)



### Docker: containers and images

- "Image" is a read-only template residing in storage and used to create a running process - the "container"
- "Repository" is a storage and access system for images
  - Can be in the cloud (DockerHub, GitLab) or local to your cluster or machine
- Example: inspect images on a local machine: "docker image Is"

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
simple_server django_import ubuntu alpine mediawiki mariadb/server nginx	latest latest latest latest latest latest	975596a4f73f	20 months ago 20 months ago 21 months ago 21 months ago 21 months ago 23 months ago 2 years ago	158MB 207MB 102MB 5.53MB 691MB 368MB 109MB



#### Docker: building images

- Building images can be conceptualized as adding layers to an underlying image
   e.g. one can start with a Ubuntu image and build an app (and its dependencies) on top
- The Docker daemon orchestrates the build based on the instructions in the "Dockerfile"
- Too many details to be covered in a short overview
- The key point is that a complete (and potentially complex) environment can be encapsulated in an image which can be preserved and ran as a container on a target system, potentially anywhere

```
Copy from the current folder

FROM ubuntu:18.04

COPY . /app

RUN make /app

CMD python /app/app.py
```



#### Docker build: a more complex example

```
&& cd /tmp/cmake-3.14.6 && ./bootstrap && make -j $(nproc) && make install \
&& mv /tmp/root /tmp/root-5-34-38 \
&& mkdir /tmp/root-build && cd /tmp/root-build \
   -DCMAKE INSTALL PREFIX=/usr/local \
   -Dpythia6 nolink=ON \
&& make install \
&& rm -fr /tmp/*
```

#### Docker: running containers

- "docker run python\_server" (can be any image available to you)
- Any number of containers can be run on a machine
- Containers can have ports open to other containers and to the host machine
- Containers can have "volumes" mapped to folders on the host
- Example: inspect containers on a local machine: "docker container ps"

```
CONTAINER ID IMAGE COMMAND CREATED STATUS PORTS d52bc1bddd84 python_server "python -m http.serv..." 12 seconds ago Up 11 seconds 8000/tcp
```

 Complete functional applications can be run by pulling images from repositories and running containers off these images



### Why use Docker?

- Building complex applications or software stacks can be difficult because of dependencies on system or 3rd party libraries or packages etc
- Two different versions of the same application may have different dependencies
- This is exacerbated when porting software from one OS/environment to another
- Docker allows for building software in a clean, well-controlled environment of your choice and then being able to run it on virtually any host
- This is valuable for software management in general and for DAP in particular
- Integration with container orchestration systems e.g. Kubernetes
- Globally used by more than 12,000 companies



# Docker: is it worth the investment of your time?

- Adoption of the container technology in industry has been overwhelming
- Wide adoption at least in the early stages in the LHC community (ALICE, ATLAS, CMS, LHCb)
- Quickly becoming a standard tool for tutorial and workshops
- Docker's cousin Singularity has achieved popularity in HEP and NP communities, with current EIC work leveraging this technology in significant ways
  - NB. PHENIX production makes use of Singularity to retain a functional legacy OS environment to ensure that results are 100% reproducible
- Staying abreast of these developments is beneficial for teams and individuals:
  - A highly desirable skill set in both science and industry
  - Capture and transfer of expertise and software within working groups and the Collaboration
  - Can be a part of the solution for Analysis Preservation
- It is a complex product but documentation is good and plentiful



#### Docker: caveats

- Need to demonstrate integration with AFS since this dependency is hard to remove
- CVS
- Database interaction
- ...a lot of technical points to be investigated
- It is understood that in the current situation Docker is mostly suitable for analysis and perhaps for its final stages
  - Too many dependencies in other parts of the workflow



#### REANA

- A framework already used by LHC experiments
- https://reanahub.io/
- Captures
  - Details of the analysis workflow by utilizing a structured description (graph/DAG)
  - Software and environment by means of containerization
- Implemented as a cluster configured to run containers and orchestrated according to formalized workflows created by users
- A test instance recently became available at BNL thanks to SDCC, initial testing for PHENIX in progress
- At a minimum, requires Docker expertise
- Still need to evaluate cost/benefit...Looks promising!



#### REANA - a real world analysis example

```
version: 0.4.0
inputs:
files:
    - config/geantSim_TrackerPerformance.py
    - config/single_particle_trackFits.py
    - script/numHitsPerTrack.C
    - script/plot_single_particle_resolutions.py
parameters:
    events: 5000
    seed: 0123456
    particle: 13
    etamin: 0
    etamax: 6
    pt: 1000 2000 5000 10000 1000000 10000000
```

```
- environment: 'gitlab-registry.cern.ch/vavolkl/fcc-ubuntu:latest'
                                                                         Image
     - fccrun.py config/geantSim TrackerPerformance.py
       -N $events -s $seed --outName muons for seeding discrete pt.root
       --singlePart --particle $particle --etaMin $etamin --etaMax $etamax
       --discretePt --pt $pt
      | tee simulation.log 2> simulation.err
     | tee plot-tracker-hits.log 2> plot-tracker-hits.err
       --inputfile muons for seeding discrete pt.root
       --outputfile single particle resolutions.root
     | tee fit.log 2> fit.err
single particle resolutions.root
     | tee plot-reconstructed-tracks.log 2> plot-reconstructed-tracks.err
```

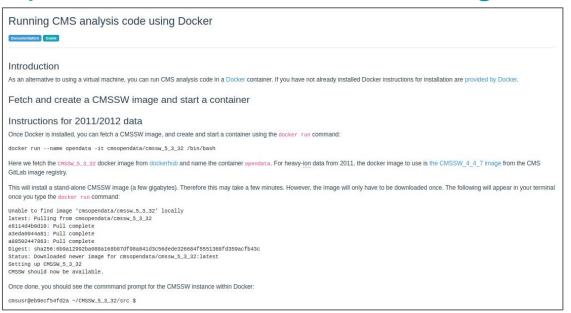
#### OpenData

- A CERN portal for capture and publishing of data samples, software and documentation
  - Consider a set of Ntuples and Docker images plus documentation provided as a cohesive package
- Initially reserved for LHC experiments
- PHENIX was given an approval and access in Fall 2020
- Storage allocated
- Currently no cost to PHENIX
- The first package/analysis is currently in the works (thanks Gabor)



# Confluence of technologies - CMS use case for Docker published on OpenData

http://opendata.cern.ch/docs/cms-guide-docker





#### PHENIX School in 2021

- The website can be leveraged as the portal to the necessary writeups/tutorials and other materials
- How much material can be made reusable for Schools, training and DAP?
- What are the prospects of creating Docker-based tools for the School?
- How much effort can the working groups contribute to the development of the School?

#### Status and Plans

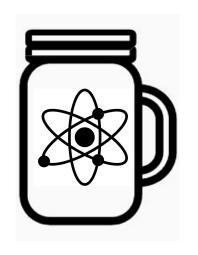
- The new durable PHENIX website has been commissioned in 2020
  - Serving as a hub for cloud resources utilized by PHENIX
  - Content is being developed and added
- Ongoing creation and uploads of curated and tagged materials to Zenodo
  - Archiving of the PHENIX theses is progressing at a good pace
  - Recent conference presentations are included
- Systematized submissions to HEPData
- Started work on OpenData items for PHENIX
- Planned adoption of REANA (pending evaluation of Docker for PHENIX)
- Main concern is lack of documented analysis use cases and vetted tutorials
  - Containerization could be a useful catalyst
- Preparation for the PHENIX School and DAP are closely related tasks so there can be economies of scale



# Backup slides



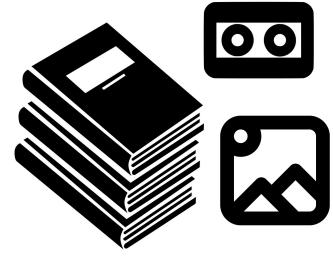
# A practical approach to the components of the Knowledge Management in PHENIX



Analysis capture



Web-based documentation



A highly-functional repository for research materials

#### The website technology

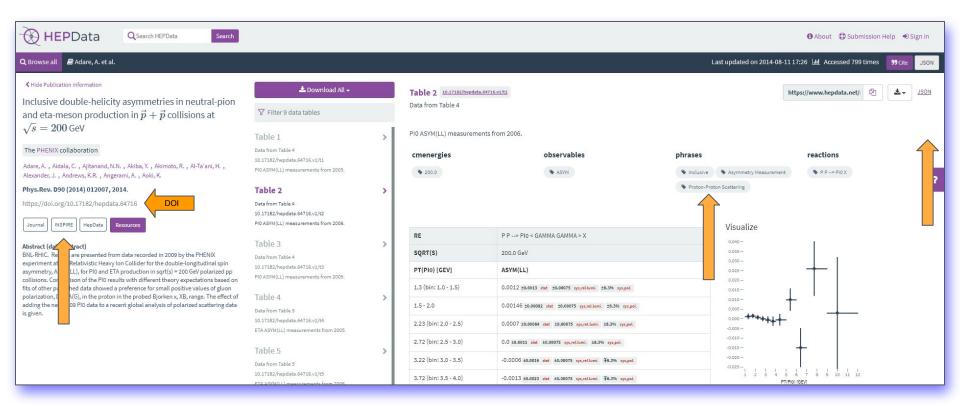
- Inspired by the websites of the HEP Software Foundation and NPPS
  - https://hepsoftwarefoundation.org/
  - https://npps.bnl.gov/
- The website is static (no DB) using the Jekyll static website generator
  - HTML is generated, not written by hand
  - Easy to contribute (Markdown, YAML) and easy to maintain
  - Data content kept separately from the layout
  - Manipulation of structured data in Jekyll makes for a compact and efficient design of pages,
     and automated content generation DB-like functionality at compile time
  - GitHub Pages for management and development + version control + Jekyll builds
  - Portability (easy to export/migrate the complete site as HTML)
  - Performance
  - Security
- The "Bootstrap" toolkit for the layouts/navigation (no custom JS/CSS needed)



# Structured data used to generate the site

```
title: Run 12
 period: 2011-2012
 coordinator: Xiaochun He, GSU.
 rhic:
     species: 'polarized p+p',
     energy: 100.2,
     lumi: '- /10 <i>pb</i><sup>-1</sup>',
     species: 'polarized p+p',
     energy: 254.9,
     lumi: '32/- <i>pb</i><sup>-1</sup>',
     species: '<sup>238</sup>U<sup>92+</sup>+<sup>238</sup>U<sup>92+</sup>',
     energy: 96.4.
     lumi: '0.2<i>nb</i><sup>-1</sup>'.
     Nevents: 1.2B/0.8B
     species: '<sup>63</sup>Cu<sup>29+</sup>+<sup>197</sup>Au<sup>79+</sup>',
     energy: 99.9+100.0,
     lumi: '5<i>nb</i><sup>-1</sup>',
     Nevents: 0.8B/8.1B
     species: '<sup>197</sup>Au<sup>79+</sup>+<sup>197</sup>Au<sup>79+</sup>',
     energy: 2.5,
     lumi: '-',
     Nevents: Very short
 ert_comment: Summary of thresholds (DAC values). Values in parentheses are for the PbG1.
 ert thresholds:
  - '02/09/12, 358208, 30(29), 31(30), 29(29), 29(25), 920, Run12pp200 - Pedestal tuned - EMCal dynamic range ~25GeV'
  - '03/20/12, 364957, 30(29), 31(30), 29(29), 29(25), 920, Run12pp510 - EMCal dynamic range ~50GeV'
  - '04/23/12, 369200, 30(29), 31(30), 29(29), 29(25), 920, Run12UU193 - EMCal dynamic range ~25GeV'
  - '05/16/12, 372155, 31(30), 32(31), 30(29), 49(45), 920, Run12CuAu200 - EMCal dynamic range ~25GeV'
```

### HEPData: an example of a PHENIX entry



#### **Open Data Definitions**

- "Canonical" data levels
- Level 1 data provides more information on published results

  Ne are here

  Level 2 data includes simplified data formats for outreach and analysis training
  - Level 3 data comprises reconstructed collision data and simulated data together with analysis-level experiment-specific software
  - Level 4 data covers basic raw data
  - Where does PHENIX stand?
    - Level 1 is covered by the current HEPData activity and auxiliary info committed to Zenodo
    - Level 2: work underway to create Ntuples illustrating analysis techniques (next slide)
    - Level 2: the Open Data Portal (under discussion)
    - Levels 3 and 4 are not practical for public access for much of the same reasons as exist in other experiments (e.g. access to calibrations and access to sites)



# The Open Data effort: annotated Ntuples (G. David)

