Data & Analysis Preservation: current work items

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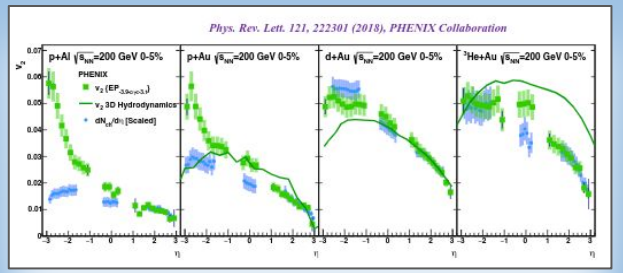


PHENIX DAP Meeting
03/25/2021

Overview

- REANA
- Docker
- Open Data
- HEPData
- Zenodo
- Website
- Analysis notes
- *Maxim on leave through April 11th (propose next meeting on April 22nd)*

REANA - a quick recap

- REANA: captures the workflow, the software, the data
  - Hence reproducibility
  - If used correctly, helps present a clear description of the computational process
- Simple, intuitive description of linear workflows in YAML
  - Can be parametrized, self-documenting
- A more complex syntax is available to arbitrary DAGs
- A very basic Web UI provided by the server
- Interaction with the system is mainly via a CLI client, which can be installed on any machine where the Python environment is available
- In addition to the CLI utility there is a full-fledged Python package which allows for potentially complex applications, scripting etc

REANA - software provisioning

- Software can be provisioned in different ways (source, images, CVMFS) depending on the needs of the calculation
  - For example, a specific version of ROOT or a Python environment can be obtained by requesting the correct image - from your chosen registry
  - Code can also be built as needed (perhaps not optimal but possible)
- All these options are available in any step of the workflow
  - e.g. the software can be provisioned differently in each step
- If the code has Docker image components, images are transparently pulled from Docker Hub or other comparable hosting service
- There is no direct mount of AFS on the worker nodes so everything needs to be staged in (CVMFS is still under discussion because if its use in EIC)
- However content from AFS can be *staged from the user's machine* if needed

REANA - the process

- Execution takes place in a sandbox
  - A process running on one of the worker nodes in the cluster
  - Scripts, macros and other software can be staged-in (provisioning)
- Status can be checked in the Web UI or with the CLI client, or with a script utilizing the Python package
- Input data is typically staged-in to the sandbox before the execution starts
  - But data handling can also be a part of the payload job
  - CVMFS
  - XRootD?
  - This will be illustrated in an example of one of the subsequent slides
- Output is staged-out upon completion
  - Once again, possible with a variety of methods

REANA - progress

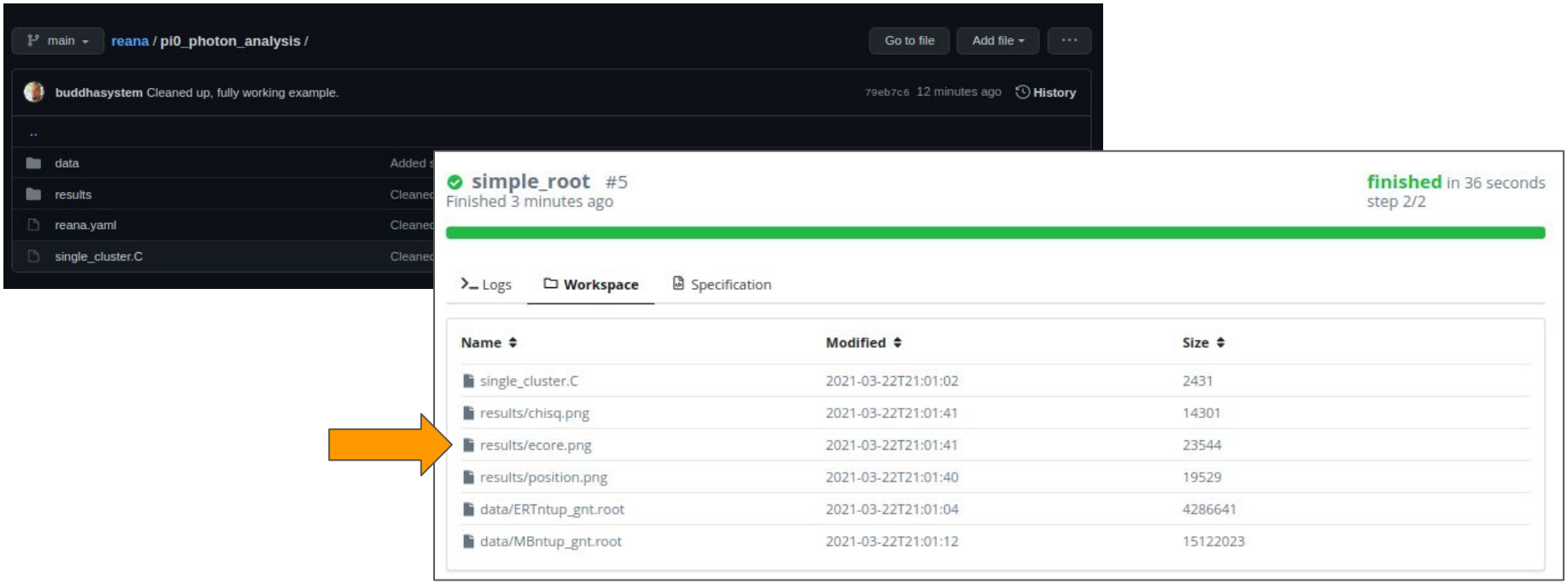
- Tested staging AFS folders (need to be careful)
- Created an official PHENIX repository for REANA workflows
  - https://github.com/PhenixCollaboration/reana
- EMCAL single-cluster example (prepared for the Open Data) *ported to REANA*
  - Committed to GitHub
  - Simple and self-contained (includes the Ntuples)
  - Suitable for the PHENIX School, can be used as a template for more complex cases
- Picked the ROOT6 version of the macro for simplicity (see the next slide)
- *Anything that is based on pure ROOT macros can be committed to REANA trivially*
- Ultimately usefulness of this exercise will depend on containerization since interesting stuff is done with the PHENIX analysis libraries
  - See comments about Docker later in this presentation

REANA - EMCAL single cluster analysis

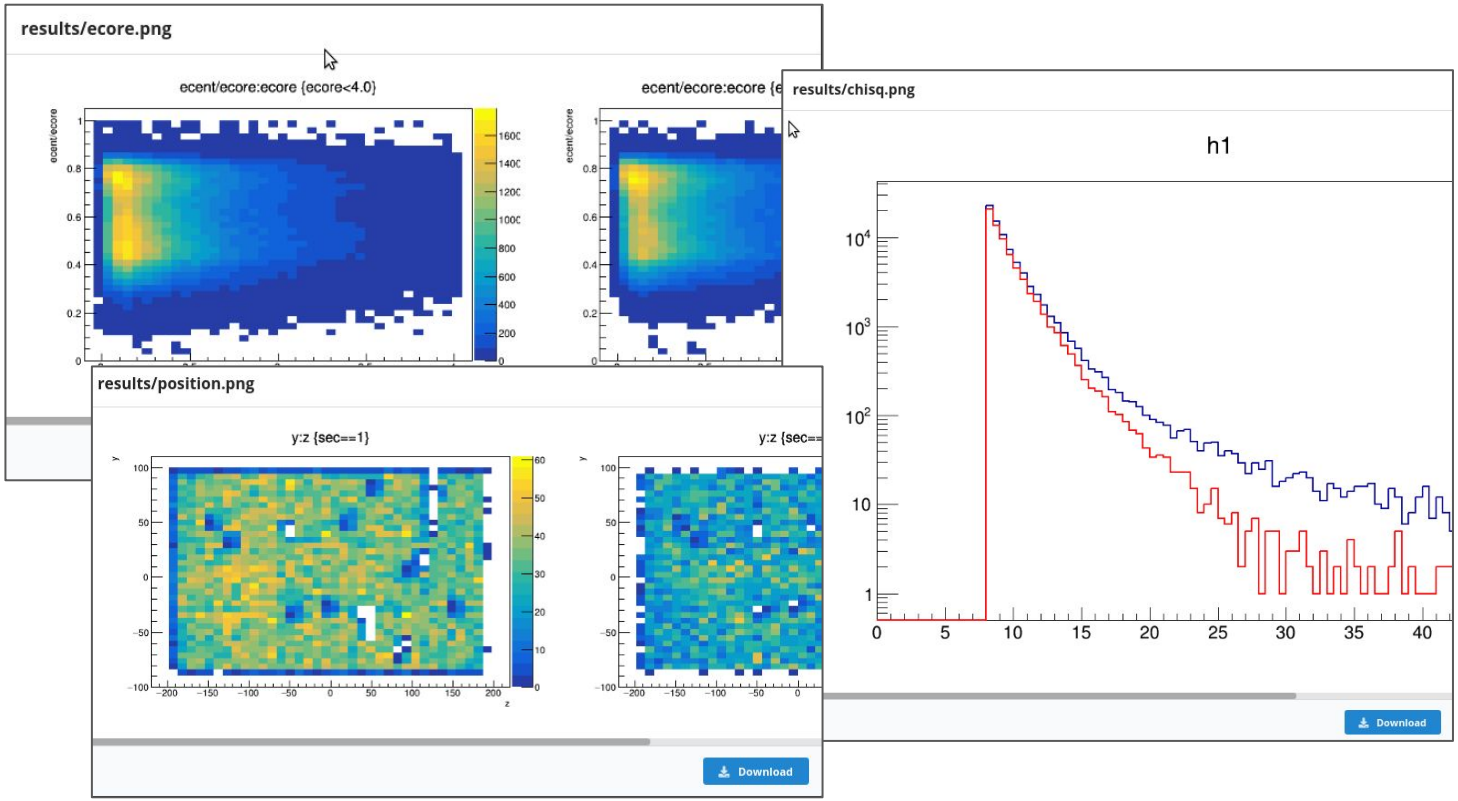
```
version: 0.0.1
inputs:
  files:
    - ./single_cluster.C
    - data/ERTntup_gnt.root
    - data/MBntup_gnt.root
workflow:
  type: serial
  specification:
    steps:
      - environment: 'rootproject/root'
        commands:
          - mkdir -p results
          - root -b -q 'single_cluster.C("position")' 'single_cluster.C("ecore")' 'single_cluster.C("chisq")'
outputs:
  files:
   - results/test.txt
```

REANA - GitHub repo, test runs

https://github.com/PhenixCollaboration/reana/tree/main/pi0_photon_analysis



REANA - results of the single cluster job



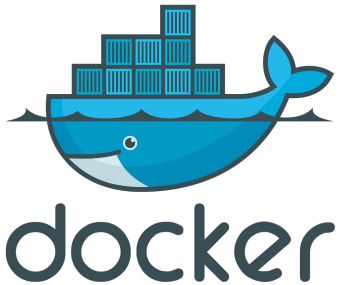
Docker: current status

- We built a functional 64-bit ROOT5/SL7 image created from source
- Hosting on Docker Hub works fine, adding any 64-bit library should be easy
- It works with C++ macros, just not the PHENIX analysis libraries at this point
- Caveat: the PHENIX software stack is built for 32-bit for legacy reasons
- Both STAR and PHENIX build there software for 32-bit
  - Both solution are tied to the respective experiment's setup

Docker: the 32-bit problem

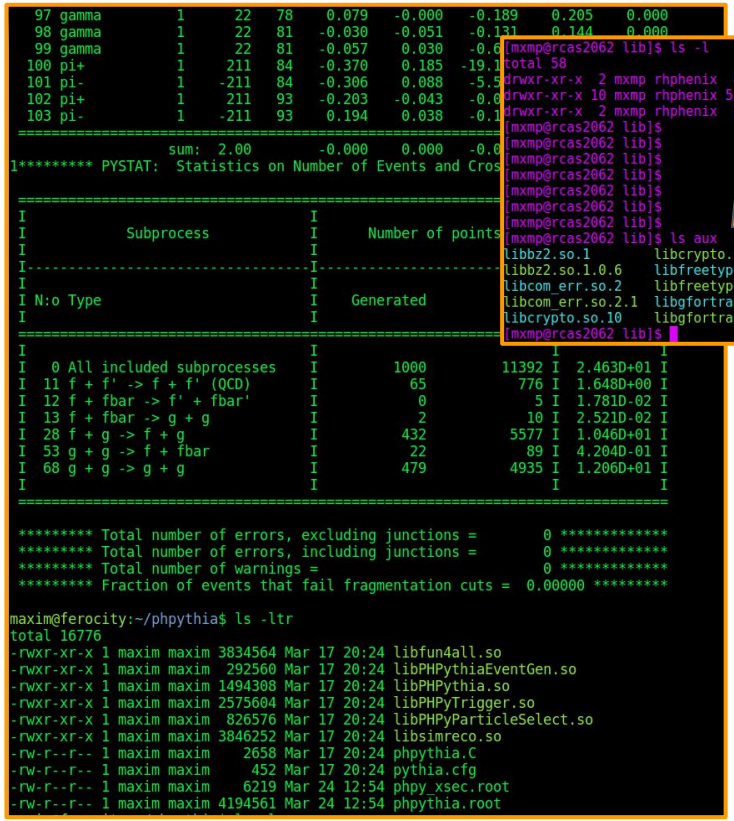
- Possible because of “multilib” feature of SL, effectively installation a parallel system of core libraries (i386 in addition to x8664) and a fairly complex setup for building ROOT via cross-compilation
  - ROOT5 available on the rcas nodes is 32-bit
- No portable procedure exists for the PHENIX stack (i.e. on someone’s workstation)
- SDCC does BNL-internal image builds but images are considered private (next slides)
- In summary, there are a lots of libraries and dependencies

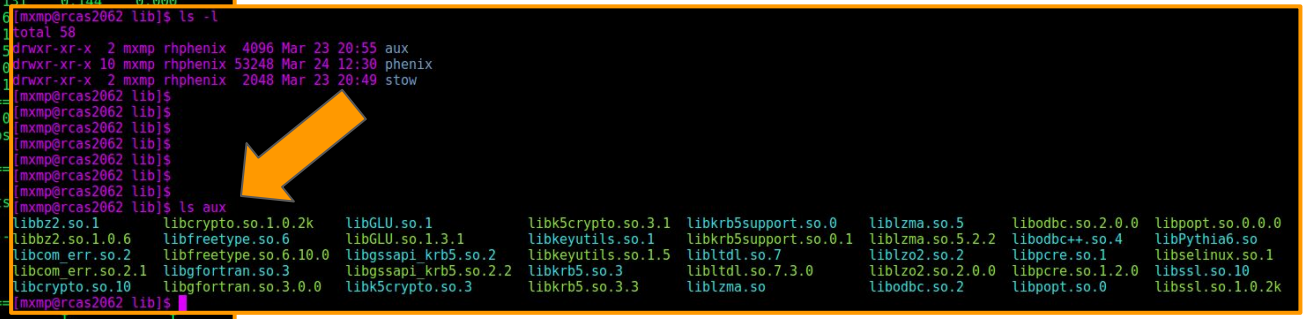
Docker: the outlook



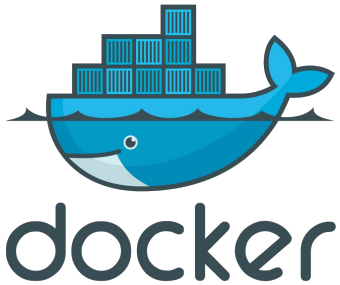
- Having a containerized PHENIX environment is a worthy goal
  - both for general DAP and REANA activities
- ***Copying libraries to a Docker image*** (as discussed before) is more involved than anticipated due to the 32-bit dependencies explained above
  - Brings in system dependencies i.e. i386 libraries that need to be identified and collected
  - *An experimental setup has been created with all the binaries managed in one place*
  - *Creating an image is the next step*
- Building this Docker image will be the focus of the DAP work for a while
- As the last option, we can try using private PHENIX/SL7 images provided by SDCC which we are not allowed to widely share for security reasons
- The issue of DB access - this only works within the BNL perimeter
  - Which analyses would be impacted if no access would be possible?

Docker - testing “phpythia” in a self-contained env

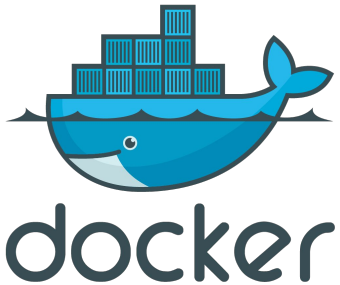




Prep work for the PHENIX image, running from a self-contained AFS area



Docker: action items



- Complete the experimental 32-bit image setup
  - i.e. the one obtained with the library collection
  - Test and understand limitations
  - If functionality adequate commit to Docker Hub
- Discuss private hosting of images at BNL which would solve the problem of the image availability and DB access
  - SDCC managing images is by far the optimal solution
  - Private registry is possible, there is a test service
  - Access mode is similar to Docker Hub i.e. images are pulled from the service
- SDCC - at some point will need to organize a meeting with a Docker focus
- Collect use cases amenable to REANization - expert help needed - Gabor, Dillon?

Open Data - the “π^0 and ɣ analysis” entry

- The companion document updated to reflect the latest round of changes
- ROOT5 and 6 versions of the macros created and tested
- Uploaded to CERN, admins notified, awaiting response
- Have enough experience at this point to create another entry, how do we get volunteers?
  - If there is a close-to-final Ntuple and some macros for event/track/cluster selection that would be a low-hanging fruit
  - Can create images complete with data if compact enough

HEPData

- A new script - to aid in formatting the errors - has been developed based on the original script developed in STAR
- Sharing OK'd by Rongrong Ma (STAR), will be credited
- Corrections by Takahito and others
- Added to the repository, will make further improvements if necessary
  - https://github.com/PhenixCollaboration/hepdata/tree/master/scripts

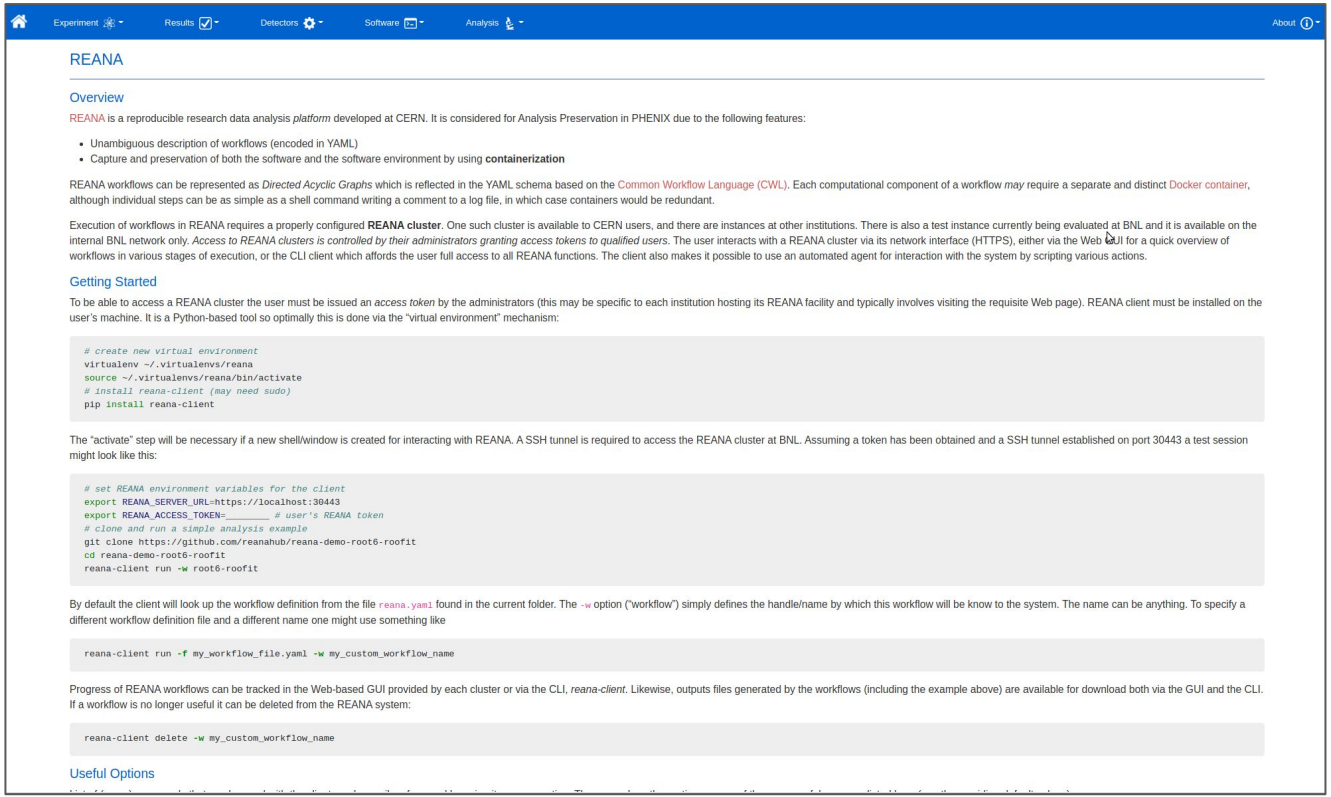
Zenodo

- More uploads of conference presentations (thanks Gabor!)
  - The “new” workflow in action, works nicely
- Correction and management of the keywords attached to Zenodo items
- A total of 340+ PHENIX items as of this week, a substantial achievement

Website

- Added/corrected conference info on the site
- 23 conferences now listed and linked on the site: webpages and Zenodo entries
- Keywords: total of 185 now
- Cleanup/improvement of links and references in a few places (DAP, Zenodo)
- Built up the REANA page (next slide) - for concise how-to information
- Pulled to production URL: https://www.phenix.bnl.gov/

Website - the updated REANA page



Analysis notes: technology downselect

- GitHub
  - More feedback from colleagues re: longevity - looks positive
  - Can start operating now
- Gitea@BNL info
  - Hosts 8 organizations at BNL with a total of 104 repositories
  - Expected lifetime: did not receive guidance or committment
- Looks like the final call should be as recommended by the EC i.e. GitHub

Plans

- *Maxim on vacation March 31st - April 11th*
  - Next meeting? Propose April 22nd (or later)
  - Docker/REANA/SDCC
  - DAP participants
- Will start hosting analysis notes on GitHub
- Docker image development is the focus area, ETA is not too clear at this point
  - There are some promising results though
- More engagement in the REANA effort?
  - Can/should start before we have containers (we already do have private ones)
  - Would consist of self-contained clean packages of macros and data