Data & Analysis Preservation: status update

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PHENIX DAP Meeting
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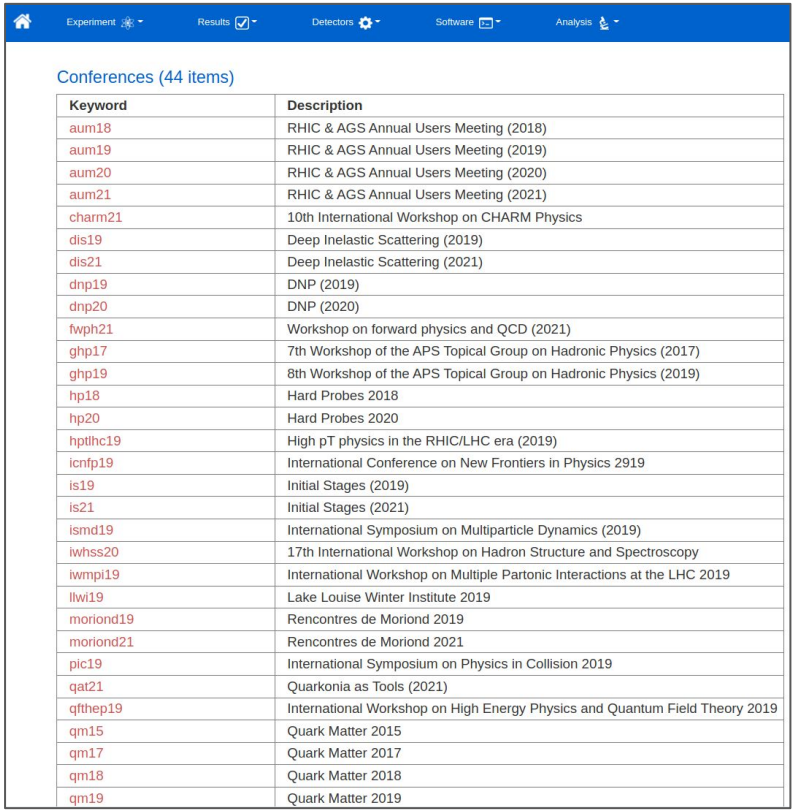
reana

PHENIX

Overview

- Zenodo+Website
- HEPData
- Docker+REANA
  - CVMFS deployment
  - Progress with realistic payloads
  - Some residual technical work might be needed
- Summary and plans

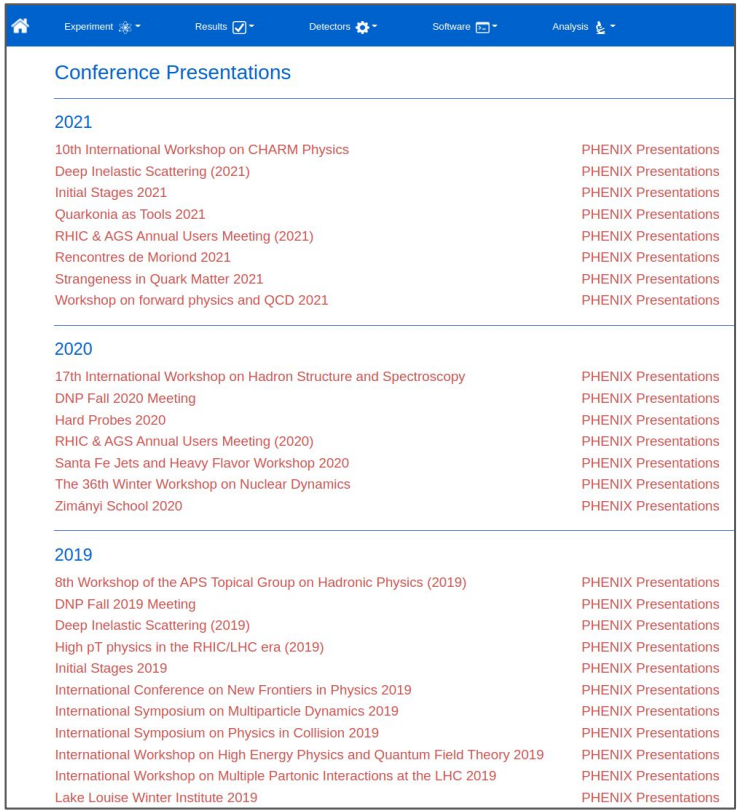
Zenodo uploads



Experiment Results Detectors Software Analysis

Conferences (44 items)

Keyword	Description
aum18	RHIC & AGS Annual Users Meeting (2018)
aum19	RHIC & AGS Annual Users Meeting (2019)
aum20	RHIC & AGS Annual Users Meeting (2020)
aum21	RHIC & AGS Annual Users Meeting (2021)
charm21	10th International Workshop on CHARM Physics
dis19	Deep Inelastic Scattering (2019)
dis21	Deep Inelastic Scattering (2021)
dnp19	DNP (2019)
dnp20	DNP (2020)
fwph21	Workshop on forward physics and QCD (2021)
ghp17	7th Workshop of the APS Topical Group on Hadronic Physics (2017)
ghp19	8th Workshop of the APS Topical Group on Hadronic Physics (2019)
hp18	Hard Probes 2018
hp20	Hard Probes 2020
hptlhc19	High pT physics in the RHIC/LHC era (2019)
icnfp19	International Conference on New Frontiers in Physics 2919
is19	Initial Stages (2019)
is21	Initial Stages (2021)
ismd19	International Symposium on Multiparticle Dynamics (2019)
iwhss20	17th International Workshop on Hadron Structure and Spectroscopy
iwmpi19	International Workshop on Multiple Partonic Interactions at the LHC 2019
llwi19	Lake Louise Winter Institute 2019
moriond19	Rencontres de Moriond 2019
moriond21	Rencontres de Moriond 2021
pic19	International Symposium on Physics in Collision 2019
qat21	Quarkonia as Tools (2021)
qfthep19	International Workshop on High Energy Physics and Quantum Field Theory 2019
qm15	Quark Matter 2015
qm17	Quark Matter 2017
qm18	Quark Matter 2018
qm19	Quark Matter 2019



Experiment Results Detectors Software Analysis

Conference Presentations

2021

10th International Workshop on CHARM Physics	PHENIX Presentations
Deep Inelastic Scattering (2021)	PHENIX Presentations
Initial Stages 2021	PHENIX Presentations
Quarkonia as Tools 2021	PHENIX Presentations
RHIC & AGS Annual Users Meeting (2021)	PHENIX Presentations
Rencontres de Moriond 2021	PHENIX Presentations
Strangeness in Quark Matter 2021	PHENIX Presentations
Workshop on forward physics and QCD 2021	PHENIX Presentations

2020

17th International Workshop on Hadron Structure and Spectroscopy	PHENIX Presentations
DNP Fall 2020 Meeting	PHENIX Presentations
Hard Probes 2020	PHENIX Presentations
RHIC & AGS Annual Users Meeting (2020)	PHENIX Presentations
Santa Fe Jets and Heavy Flavor Workshop 2020	PHENIX Presentations
The 36th Winter Workshop on Nuclear Dynamics	PHENIX Presentations
Zimányi School 2020	PHENIX Presentations

2019

8th Workshop of the APS Topical Group on Hadronic Physics (2019)	PHENIX Presentations
DNP Fall 2019 Meeting	PHENIX Presentations
Deep Inelastic Scattering (2019)	PHENIX Presentations
High pT physics in the RHIC/LHC era (2019)	PHENIX Presentations
Initial Stages 2019	PHENIX Presentations
International Conference on New Frontiers in Physics 2019	PHENIX Presentations
International Symposium on Multiparticle Dynamics 2019	PHENIX Presentations
International Symposium on Physics in Collision 2019	PHENIX Presentations
International Workshop on High Energy Physics and Quantum Field Theory 2019	PHENIX Presentations
International Workshop on Multiple Partonic Interactions at the LHC 2019	PHENIX Presentations
Lake Louise Winter Institute 2019	PHENIX Presentations

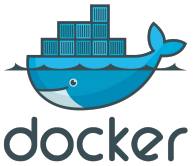
Zenodo+Website

- Uploads ongoing (thanks Gabor)
  - Total of 44 conferences included
  - 2019, 2020 and 2021 are all covered
  - Six more conferences since last report + relevant keywords
- (Some) School'21 materials were added as well
  - DAP: 3 sets of slides also added to the PHENIX GitHub repo
- REANA page corrections

HEPData

- Master spreadsheet updated
- PPG071 (revision), PPG115 finalized
- Other active items in the pipeline: 026, 201, 238

Docker: a recap (one last time)



- The core problem for containerizing the PHENIX software:
  - *PHENIX software components evolved over ~20 years accumulating dependencies*
  - *Large number of dependencies on packages installed on the SDCC cluster resulted in two subsidiary issues*
    - *No “clean build” procedure available - too many components to be covered*
    - *Large size of the sum of binaries - too large for Docker*
  - *An attempt to build a smaller “custom image” by chasing down and isolating dependencies proved very time-consuming and not completely reliable*

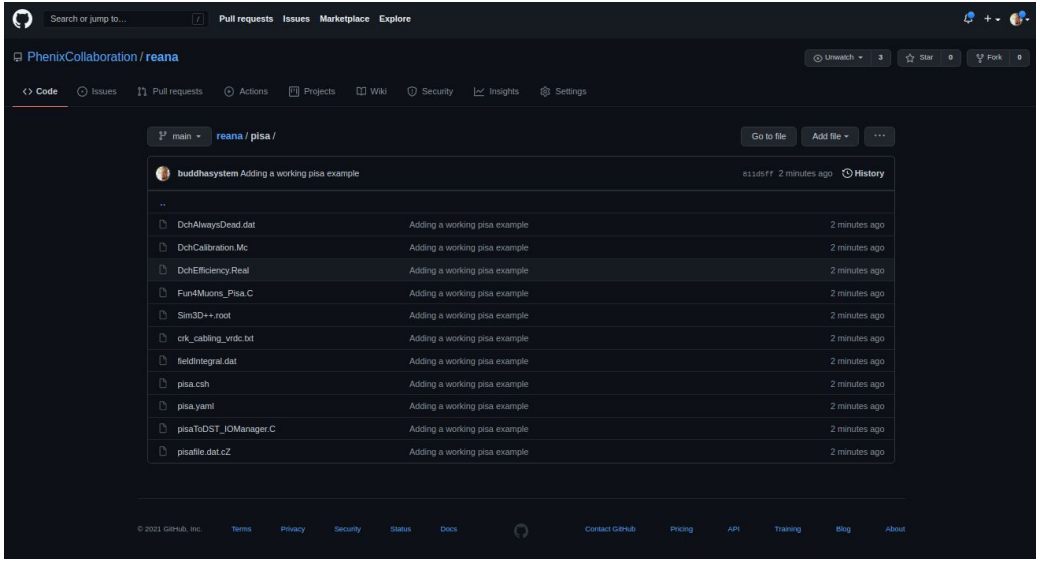
- The SDCC-provided images were developed in parallel - now the preferred option
  - *The idea is to have a complete snapshot of SDCC + PHENIX stack deployed to CVMFS*
  - *...resulting in a compact image + 30GB of binaries available on demand*
  - *...see next slide about CVMFS*

CVMFS

- The CernVM File System (originally developed to support the CERN VM project)
- A scalable, reliable and low-maintenance software distribution service
- The client uses outgoing HTTP connections only (no firewall issues)
- From the user perspective it is somewhat like read-only AFS
  - Key: globally visible (if mounted), can be used on clusters like REANA anywhere
  - Only admins can deploy to CVMFS
  - Can have a POSIX interface via FUSE (i.e. can browse it like most filesystems)
- Widely used in HEP everywhere
- Example of setting an environment variable in a user script:
  setenv OFFLINE_MAIN /cvmfs/phenix.sdcc.bnl.gov/x8664_sl7/release/release_new/new

REANA: recent progress

- REANA tutorials during the school went well
- SDCC made a few iterations of the PHENIX image with CVMFS-based provisioning of binaries - can be used both in REANA and Singularity
- The goal now is to expand validation with realistic macros and understand potential problems (e.g recently resolved the database driver issue)
- Added working examples to the repo
  - PISA to DST
  - Run 16 QA “prod_output”



REANA “workspaces”

- The usual facility-wide filesystems are not visible from the worker nodes in the REANA cluster (i.e. no access to gpfs, nfs, afs etc)
- All the files needed by a workflow are meant to be staged in and staged out by the REANA client, before and after the workflow execution - and they reside in the scratch space known as “workspace”
- Each workspace is private for each instance of workflow
- The user can browse the workspaces using the Web browser and also the CLI client
- Example - if you create multiple workflows under the same tag “my_workflow”, reana will instantiate instances indexed by an integer i.e. my_workflow.1, my_workflow.2, my_workflow.3 etc. Still, each instance will only have access to its own workspace.

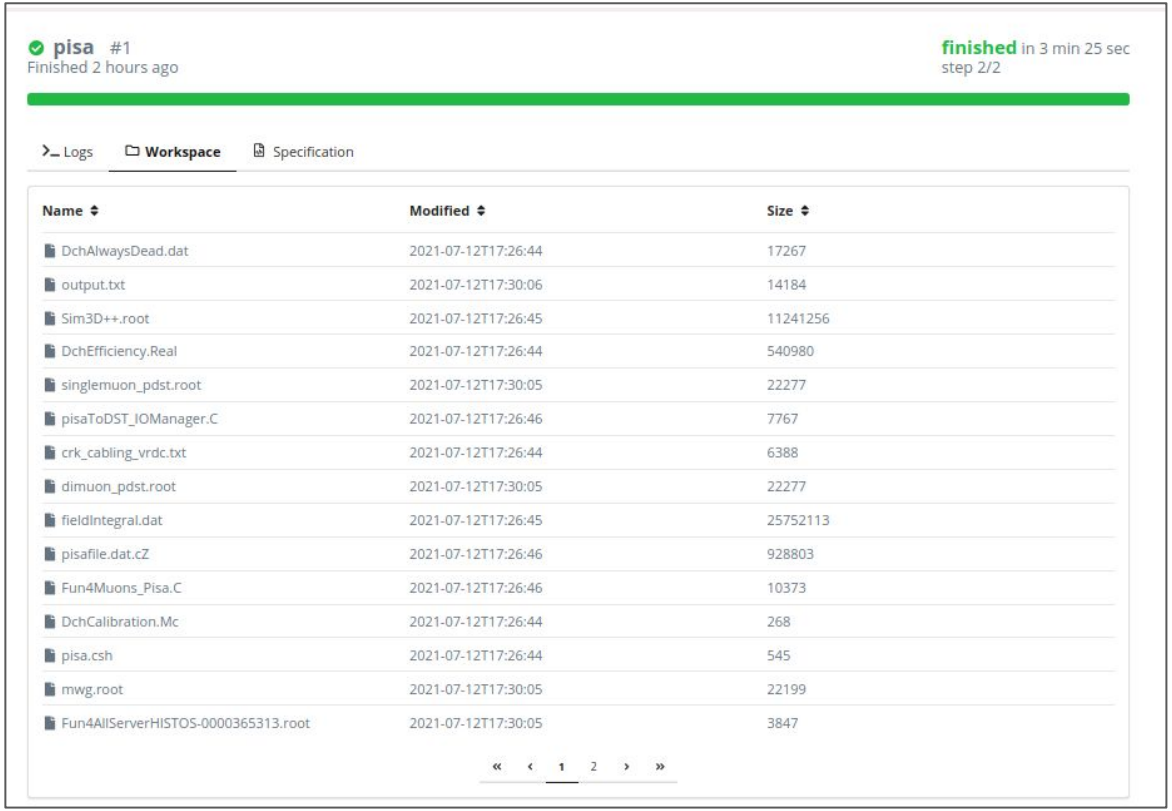
REANA I/O

- When staging in files from a “/” path rather than the current directory, a complex path will be created, relative to the workspace
  - /afs/rhic.bnl.gov/phenix/etc/odbc.ini ⇨ ./afs/rhic.bnl.gov/phenix/etc/odbc.ini
  - This pattern will also apply when staging data directly from GPFS
- For multi-GB upload packages the transfer will take a few minutes in our current REANA environment
- A complete folder can be staged in using the “directory” attribute in YAML
  - Care must be taken since directories can be quite large - beware AFS may take forever, and the overall quota may be exceeded (TBD)

REANA I/O (cont'd)

- The contents of a workspace can be updated as needed w/o having to create a completely new one - workflows can be restarted with new/updated data if needed
  - This is useful when there is a large amount of data already staged and the user needs to make a correction
- If the outputs are correctly defined, it takes a simple "download" command to get the results back to your workstation
- Alternatively, every individual file in the workspace can be downloaded if needed using the Web UI (through the browser)

REANA: “PISA to DST workspace” example

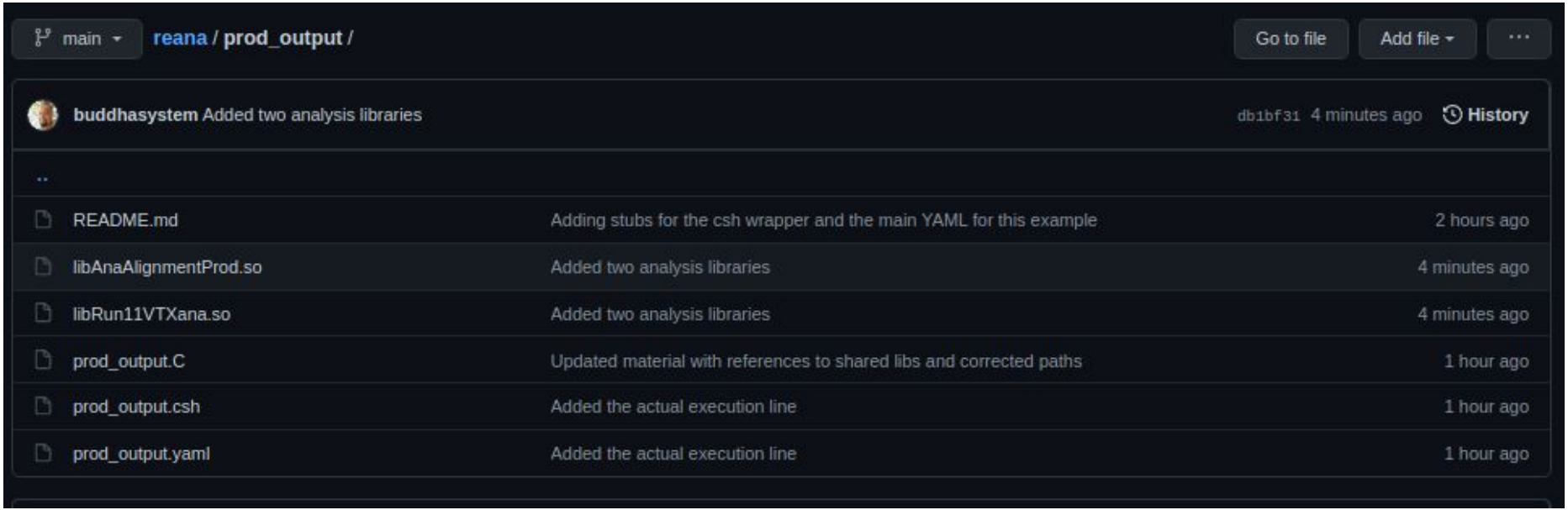



```
File Edit Options Buffers Tools Help
version: 0.0.1
inputs:
  parameters:
    odbc:
  files:
    - /afs/rhic.bnl.gov/phenix/etc/odbc.ini
#    - /afs/rhic.bnl.gov/phenix/etc/odbc.ini.phnxdbrcf2.orig
    - ./pisa.csh
    - ./DchCalibration.Mc
    - ./DchEfficiency.Real
    - ./DchAlwaysDead.dat
    - ./crk_cabling_vrdc.txt
    - ./fieldIntegral.dat
    - ./Sim3D++.root
    - ./pisafile.dat.cZ
    - ./pisaToDST_IOManager.C
    - ./Fun4Muons_Pisa.C
workflow:
  type: serial
  specification:
    steps:
      - environment: 'registry.sdcc.bnl.gov/sdcc-fabric/rhic_sl7_ext:1.3'
        commands:
        - chmod +x ./pisa.csh
        - ./pisa.csh > output.txt
outputs:
  files:
    - output.txt
    - singlemuon_pdst.root
    - dimuon_pdst.root
    - mwg.root
    - Fun4AllServerHISTOS-0000365313.root
```

Files declared in the “outputs” section can be easily downloaded using the reana client: reana-client download -w pisa

REANA: run16 QA example on GitHub

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



REANA submission for run16 QA

```
version: 0.0.1
inputs:
  files:
    - /afs/rhic.bnl.gov/phenix/etc/odbc.ini
    - ./prod_output.csh
    - ./prod_output.C
    - ./libAnaAlignmentProd.so # any analysis-specific shared libraries can be organized optimally as folders etc
    - ./libRun11VTXana.so
    - /phenix/crs/agg/run16/run16AuAu_200GeV_CA_pro111_agg/CNT_MB/CNT_MB_run16AuAu_200GeV_CA_pro111-0000459208-9000.root
    - /phenix/crs/agg/run16/run16AuAu_200GeV_CA_pro111_agg/DST_SVX_MB/DST_SVX_MB_run16AuAu_200GeV_CA_pro111-0000459208-9000.root
    - /phenix/crs/agg/run16/run16AuAu_200GeV_CA_pro111_agg/DST_EVE_MB/DST_EVE_MB_run16AuAu_200GeV_CA_pro111-0000459208-9000.root
workflow:
  type: serial
  specification:
    steps:
      - environment: 'registry.sdcc.bnl.gov/sdcc-fabric/rhic_sl7_ext:1.3'
        commands:
        - chmod +x ./prod_output.csh
        - mv ./phenix/crs/agg/run16/run16AuAu_200GeV_CA_pro111_agg/*/*.root .
        - rm -fr ./phenix
        - ls > output.txt
        - ./prod_output.csh >> output.txt
outputs:
  files:
    - output.txt
    - test_459208.root
```

Automating REANA submission

- If the number of input/output files is large, manual tweaking of the YAML file for REANA submission becomes tedious and error prone
- An initial simple prototype script has been created (and can be vastly improved) which allows to automatically fill out a template with blocks in input and output file definitions; based on the Jinja2 template engine which allows for rich logic to be included in the templates (inheritance, conditions, loops etc)
- Can be extended to handle wildcards in a folder, based on some criteria
  - e.g. file0001-9999 can be included as inputs, and output names can be inferred
  - Need some use cases to move forward with implementation; what patterns in folder names and filenames need to be parsed?
- Total storage on the REANA cluster is limited so scripting will be needed for staging the data in and out in any case, and will need to be mindful of quotas

REANA templates and the helper script

master ▾ devstash / jinja2 / templates / reana_template.yaml — Go to file

buddhasystem Improved the template — Latest commit d9cba44 41 minutes ago — History

1 contributor

15 lines (15 sloc) | 255 Bytes — Raw | Blame

```
version: 0.8.1
inputs:
  files:
{{input_files}}
workflow:
  type: serial
  specification:
    steps:
      - environment: {{environment}}
        commands:
        - chmod +x ./pisa.csh
        - ./pisa.csh > output.txt
outputs:
  files:
{{output_files}}
```

```
maxim@ferocity:~/devstash/jinja2$ ./run.py --help
usage: run.py [-h] [-t TEMPLATE] [-i INPUT_FILES] [-o OUTPUT_FILES]
              [-e ENVIRONMENT]

optional arguments:
  -h, --help            show this help message and exit
  -t TEMPLATE, --template TEMPLATE
                        template, defaults to reana_template.yaml
  -i INPUT_FILES, --input_files INPUT_FILES
                        YAML formatted list of input files, defaults to
                        input_files.yaml
  -o OUTPUT_FILES, --output_files OUTPUT_FILES
                        YAML formatted list of output files, defaults to
                        input_files.yaml
  -e ENVIRONMENT, --environment ENVIRONMENT
                        the image to use, defaults to
                        'registry.sdcc.bnl.gov/sdcc-fabric/rhic_sl7_ext:1.3'
maxim@ferocity:~/devstash/jinja2$
```

REANA submission: a possible design

- Create a base template specific to a particular analysis
  - e.g. references to specific macros and conditions, all local to the current folder
  - This makes the analysis case self-contained and suitable for preservation
  - Input files (and references) are not included in the template (can be restored later if deleted)
- Have a companion script generate lists of inputs (and if needed outputs) based on wildcards or other similar criteria
- Have the template extrapolation script generate REANA submission files for large groups of inputs; record groupings in a unified log
- Submit workflows to REANA, perhaps with an additional wrapper
- Monitor execution and download outputs before staging in more data

REANA roadmap

- There has been a substantial investment of effort invested in the images and REANA
- Conservatively 80% of work on tuning Docker images has been done
- Simple - but realistic - PHENIX examples work
- To start seeing dividends of this work we need wider community engagement - really the key to completing this work area and making it meaningful
- Should we organize a REANA seminar for the PHENIX community, as a follow up to the School tutorials?
- Can we identify ~2 PPGs who can be asked to “reanify” some parts of their analysis?
  - There are some direct benefits for the groups (self-documented reproducible procedures)
  - REANA take-up can be facilitated by providing templates for submission files

Summary

- Complete Docker images - good progress has been made
  - Initial REANA testing promising
  - Focus: setting up REANA environments for various use cases + automation
  - Participation of people doing analyses is crucial
  - Suggestions for use cases are welcome and needed
- HEPData, steady state effort (take some “pinging” to keep things moving)
- Presentations at the School, AUM and DPHEP were well received
- The PHENIX section of the NPP PAC is very positive, including the DAP mention
- Due to Gabor’s effort there is progress in migration of conference materials to Zenodo, with curated keywords - dependency on the legacy catalog is reduced
- Any new ideas re: new OpenData entries?