Reproducible high energy physics analyses

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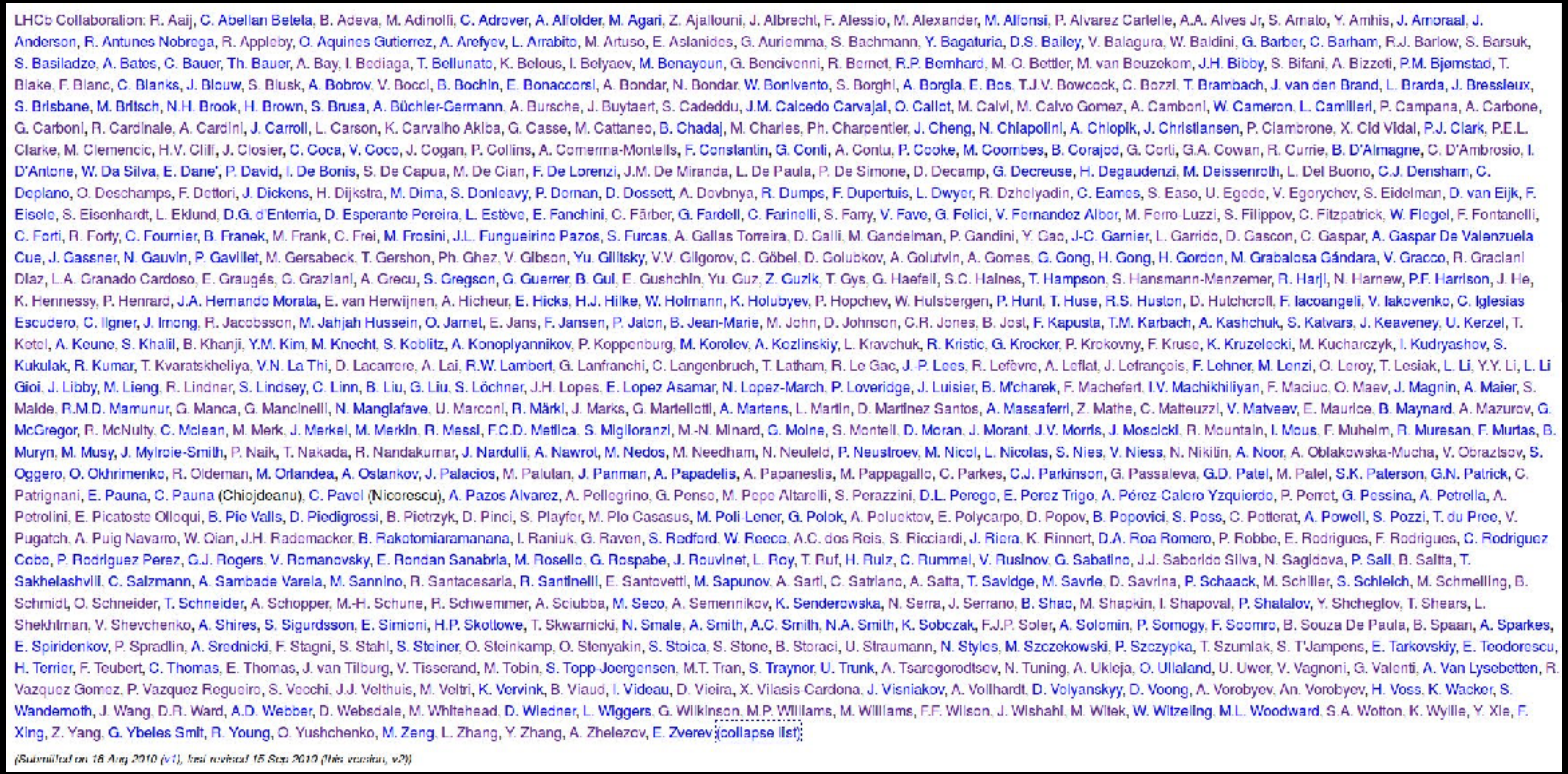
CERN

CS3 2018 - Workshop on Cloud Storage Synchronization and Sharing Services, Kraków

Knowledge
Environment
Software
Data

High turnover of researchers



LHCb Collaboration: R. Aaij, C. Abellan Beteta, B. Adeva, M. Adinolfi, C. Adrover, A. Affolder, M. Agari, Z. Ajaltouni, J. Albrecht, F. Alessio, M. Alexander, M. Alfonsi, P. Alvarez Cartelle, A.A. Alves Jr, S. Amato, Y. Amhis, J. Amoraal, J. Anderson, R. Antunes Nobrega, R. Appleby, O. Aquines Gutierrez, A. Arefyev, L. Arrabito, M. Artuso, E. Aslanides, G. Auriemma, S. Bachmann, Y. Bagaturia, D.S. Bailey, V. Balagura, W. Baldini, G. Barber, C. Barham, R.J. Barlow, S. Barsuk, S. Basiladze, A. Bates, C. Bauer, Th. Bauer, A. Bay, I. Bediaga, T. Bellunato, K. Belous, I. Belyaev, M. Benayoun, G. Bencivenni, R. Bernet, R.P. Bernhard, M. O. Bettler, M. van Beuzekom, J.H. Bibby, S. Bifani, A. Bizzeti, P.M. Bjørnstad, T. Blake, F. Blanc, C. Blanks, J. Blouw, S. Blusk, A. Bobrov, V. Bocci, B. Bochin, E. Bonaccorsi, A. Bondar, N. Bondar, W. Bonivento, S. Borghi, A. Borgia, E. Bos, T.J.V. Bowcock, C. Bozzi, T. Brambach, J. van den Brand, L. Brarda, J. Bressieux, S. Brisbane, M. Britsch, N.H. Brook, H. Brown, S. Brusa, A. Büchler-Germann, A. Bursche, J. Buytaert, S. Cadeddu, J.M. Caicedo Carvajal, O. Callot, M. Calvi, M. Calvo Gomez, A. Camboni, W. Cameron, L. Camilleri, P. Campana, A. Carbone, G. Carboni, R. Cardinale, A. Cardini, J. Carroll, L. Carson, K. Carvalho Akiba, G. Casse, M. Cattaneo, B. Chadaj, M. Charles, Ph. Charpentier, J. Cheng, N. Chiapolini, A. Chlopik, J. Christiansen, P. Ciambrone, X. Cid Vidal, P.J. Clark, P.E.L. Clarke, M. Clemencic, H.V. Cliff, J. Closier, C. Coca, V. Coco, J. Cogan, P. Collins, A. Comerma-Montells, F. Constantin, G. Conti, A. Contu, P. Cooke, M. Coombes, B. Corajod, G. Corti, G.A. Cowan, R. Currie, B. D'Almagne, C. D'Ambrosio, I. D'Antone, W. Da Silva, E. Dane', P. David, I. De Bonis, S. De Capua, M. De Cian, F. De Lorenzi, J.M. De Miranda, L. De Paula, P. De Simone, D. Decamp, G. Decreuse, H. Degaudenzi, M. Deissenroth, L. Del Buono, C.J. Densham, C. Deplano, O. Deschamps, F. Dettori, J. Dickens, H. Dijkstra, M. Dima, S. Donleavy, P. Dornan, D. Dossett, A. Dovbnya, R. Dumps, F. Dupertuis, L. Dwyer, R. Dzhelyadin, C. Eames, S. Easo, U. Egede, V. Egorychev, S. Eidelman, D. van Eijk, F. Eisele, S. Eisenhardt, L. Eklund, D.G. d'Enterria, D. Esperante Pereira, L. Estève, E. Fanchini, C. Färber, G. Fardell, C. Farinelli, S. Farry, V. Fave, G. Felici, V. Fernandez Albor, M. Ferro-Luzzi, S. Filippov, C. Fitzpatrick, W. Flegel, F. Fontanelli, C. Forti, R. Forty, C. Fournier, B. Franek, M. Frank, C. Frei, M. Frosini, J.L. Fungueirino Pazos, S. Furcas, A. Gallas Torreira, D. Galli, M. Gandelman, P. Gandini, Y. Gao, J-C. Garnier, L. Garrido, D. Gascon, C. Gaspar, A. Gaspar De Valenzuela Cue, J. Gassner, N. Gauvin, P. Gavillet, M. Gersabeck, T. Gershon, Ph. Ghez, V. Gibson, Yu. Gilitsky, V.V. Gligorov, C. Göbel, D. Golubkov, A. Golutvin, A. Gomes, G. Gong, H. Gong, H. Gordon, M. Grabalosa Gándara, V. Gracco, R. Graciani Diaz, L.A. Granado Cardoso, E. Graugés, G. Graziani, A. Grecu, S. Gregson, G. Guerrer, B. 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Le Gac, J.-P. Lees, R. Lefèvre, A. Leflat, J. Lefrançois, F. Lehner, M. Lenzi, O. Leroy, T. Lesiak, L. Li, Y.Y. Li, L. Li Gioi, J. Libby, M. Lieng, R. Lindner, S. Lindsey, C. Linn, B. Liu, G. Liu, S. Löchner, J.H. Lopes, E. Lopez Asamar, N. Lopez-March, P. Loveridge, J. Luisier, B. M'charek, F. Machefert, I.V. Machikhiliyan, F. Maciuc, O. Maev, J. Magnin, A. Maier, S. Malde, R.M.D. Mamunur, G. Manca, G. Mancinelli, N. Mangiafave, U. Marconi, R. Märki, J. Marks, G. Martellotti, A. Martens, L. Martin, D. Martinez Santos, A. Massaferri, Z. Mathe, C. Matteuzzi, V. Matveev, E. Maurice, B. Maynard, A. Mazurov, G. McGregor, R. McNulty, C. Mclean, M. Merk, J. Merkel, M. Merkin, R. Messi, F.C.D. Metlica, S. Miglioranzi, M.-N. Minard, G. Moine, S. Monteil, D. Moran, J. Morant, J.V. Morris, J. Moscicki, R. Mountain, I. Mous, F. Muheim, R. Muresan, F. Murtas, B. Muryn, M. Musy, J. Mylroie-Smith, P. Naik, T. Nakada, R. Nandakumar, J. Nardulli, A. Nawrot, M. Nedos, M. Needham, N. Neufeld, P. 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Rinnert, D.A. Roa Romero, P. Robbe, E. Rodrigues, F. Rodrigues, C. Rodriguez Cobo, P. Rodriguez Perez, G.J. Rogers, V. Romanovsky, E. Rondan Sanabria, M. Rosello, G. Rospabe, J. Rouvinet, L. Roy, T. Ruf, H. Ruiz, C. Rummel, V. Rusinov, G. Sabatino, J.J. Saborido Silva, N. Sagidova, P. Sail, B. Saitta, T. Sakhelashvili, C. Salzmann, A. Sambade Varela, M. Sannino, R. Santacesaria, R. Santinelli, E. Santovetti, M. Sapunov, A. Sarti, C. Satriano, A. Satta, T. Savidge, M. Savrie, D. Savrina, P. Schaack, M. Schiller, S. Schleich, M. Schmelling, B. Schmidt, O. Schneider, T. Schneider, A. Schopper, M.-H. Schune, R. Schwemmer, A. Sciubba, M. Seco, A. Semennikov, K. Senderowska, N. Serra, J. Serrano, B. Shao, M. Shapkin, I. Shapoval, P. Shatalov, Y. Shcheglov, T. Shears, L. Shekhtman, V. Shevchenko, A. Shires, S. Sigurdsson, E. Simioni, H.P. Skottowe, T. Skwarnicki, N. Smale, A. Smith, A.C. Smith, N.A. Smith, K. Sobczak, F.J.P. Soler, A. Solomin, P. Somogy, F. Soomro, B. Souza De Paula, B. 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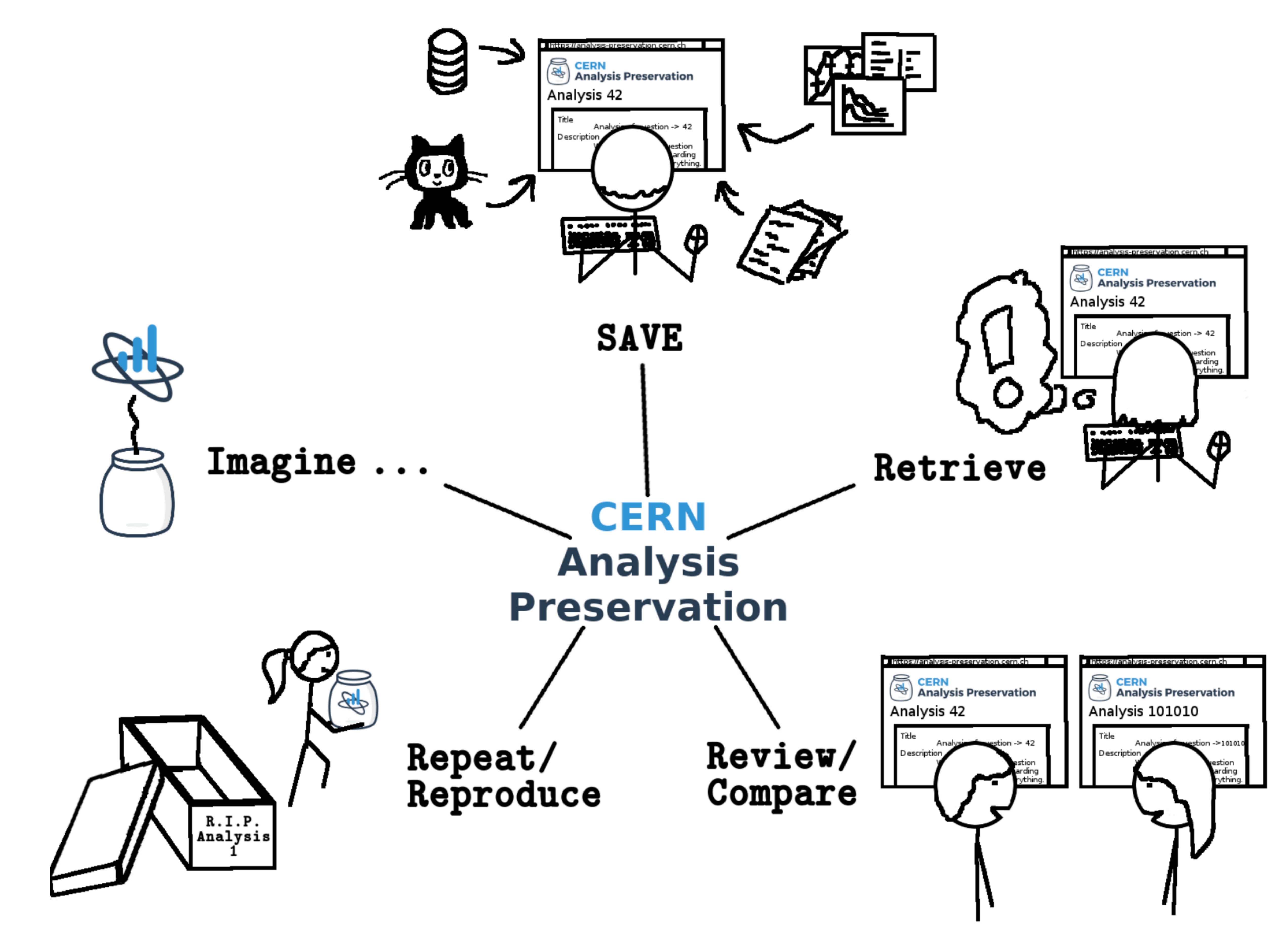
Yang, G. Ybeles Smit, R. Young, O. Yushchenko, M. Zeng, L. Zhang, Y. Zhang, A. Zhelezov, E. Zverev (collapse list)

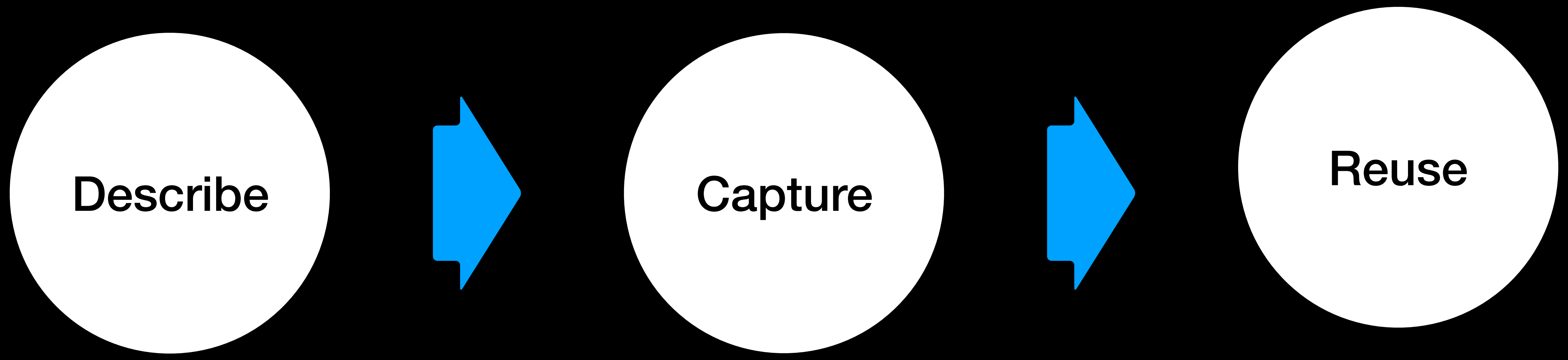
(Submitted on 16 Aug 2010 (v1), last revised 15 Sep 2010 (this version, v2))

"Particle Physics author lists change with time. Here that of the first @LHCbExperiment paper in 2010. Violet: still in LHCb. Blue: left LHCb" - @PKoppenburg

Use cases


CERN
Analysis
Preservation
SAVE
Imagine ...
Retrieve
Repeat/
Reproduce
Review/
Compare
CERN
Analysis Preservation
Analysis 42
Analysis 101010
Title
Description
R.I.P.
Analysis
1

Three pillars



Describe

Capture

Reuse

CERN Analysis Preservation

A platform for **preserving knowledge** and **assets** of an individual physics analysis

Capturing the elements needed to **understand** and **rerun** an analysis even several years after

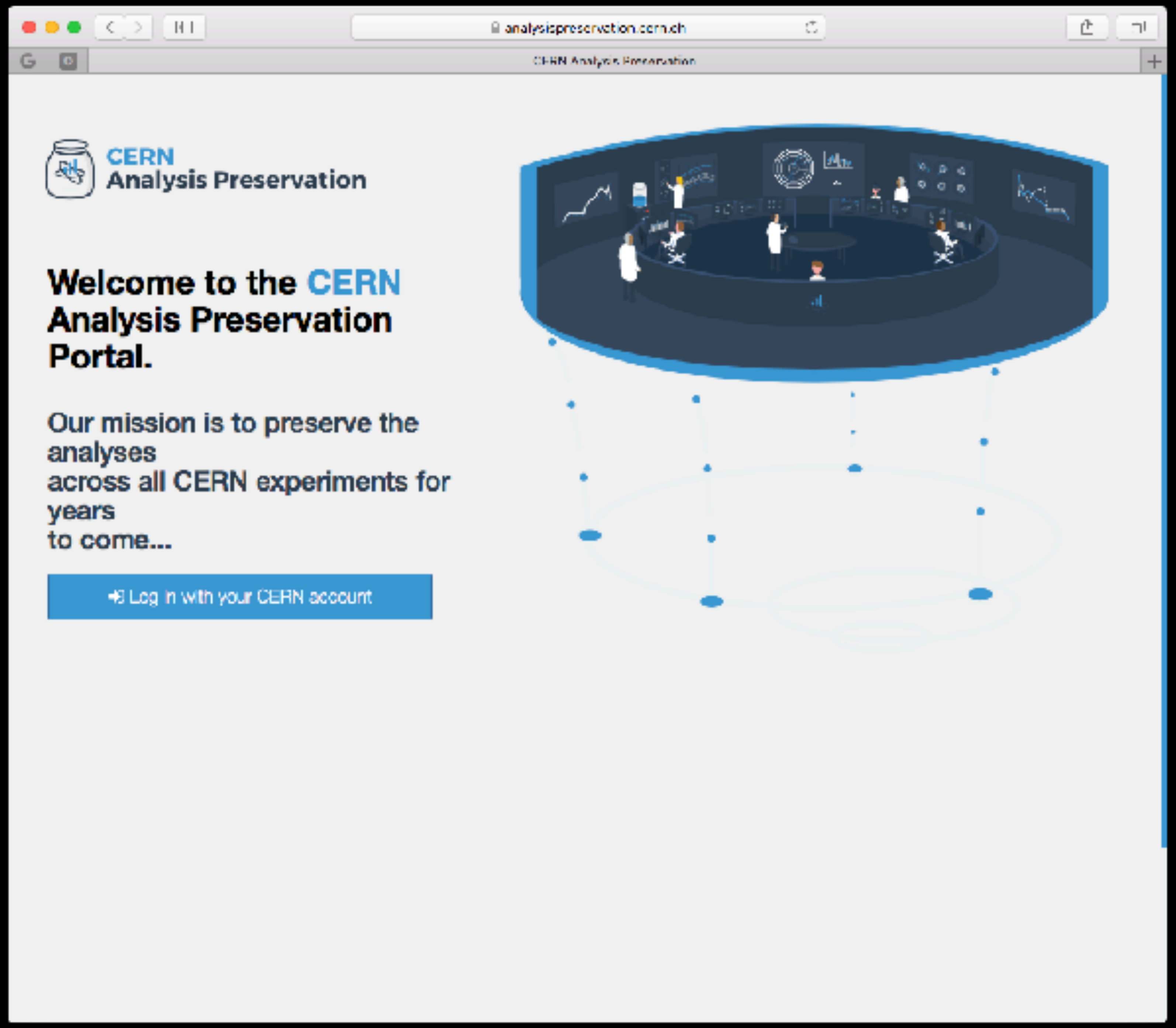
Advanced **search** for high-level physics information

Applying standard **collaboration access restrictions**

Describe

Capture

CERN Analysis Preservation



analysispreservation.cern.ch

CERN Analysis Preservation

CERN Analysis Preservation

Welcome to the CERN Analysis Preservation Portal.

Our mission is to preserve the analyses
across all CERN experiments for years
to come...

INVENIO

- JSONSchema
- W3C DCAT
- domain-specific-fields
- collaborative capabilities
- grabbing from Git, HTTP, XRootD
- powerful search

Reuse

REANA: Reusable Analyses

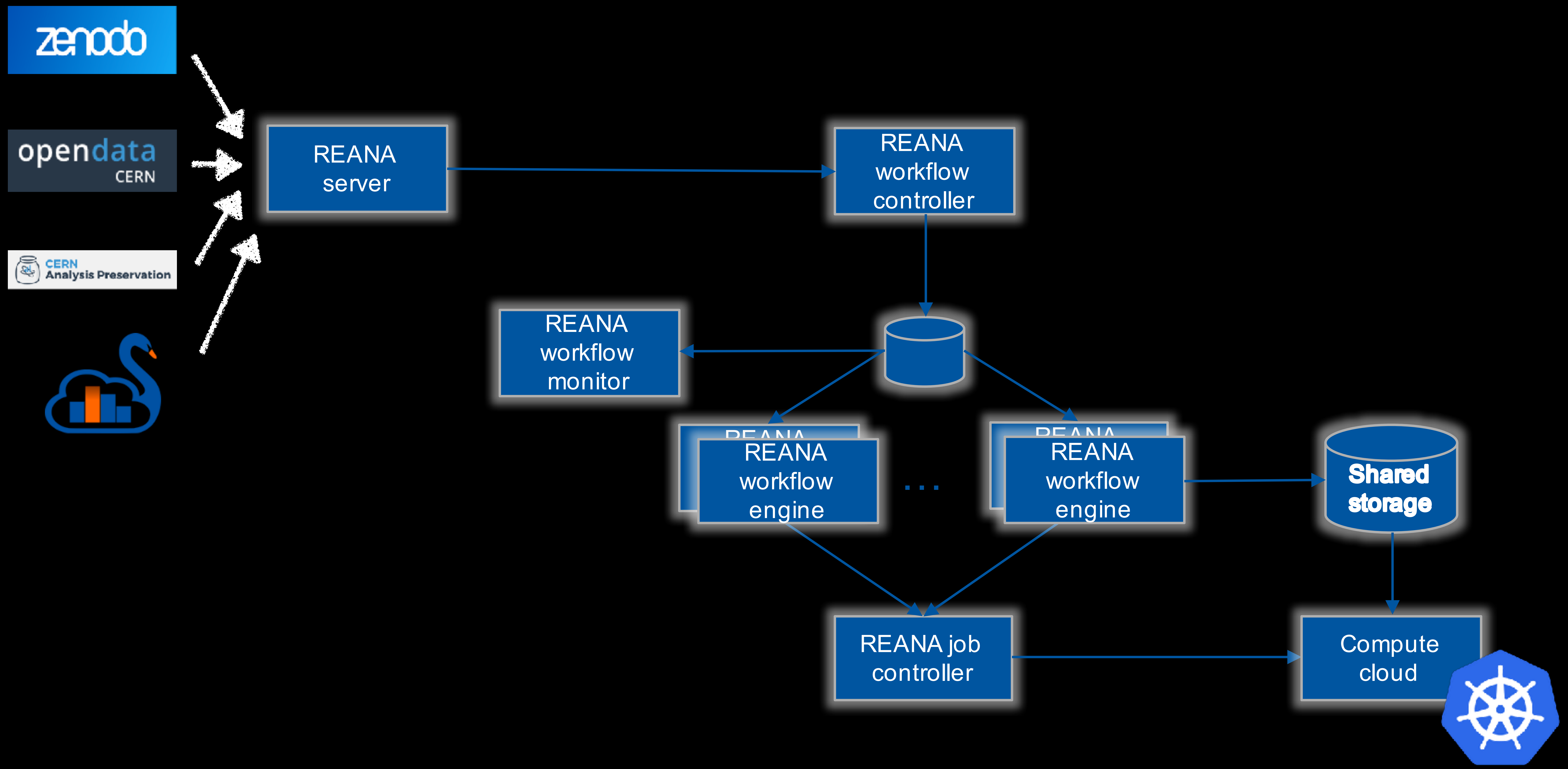
Born as part of the CERN Analysis Preservation framework

A platform which enables the **reusability** of physics analysis

Based in **cloud technologies**

Following the **12-factor application pattern**

Technology: REANA

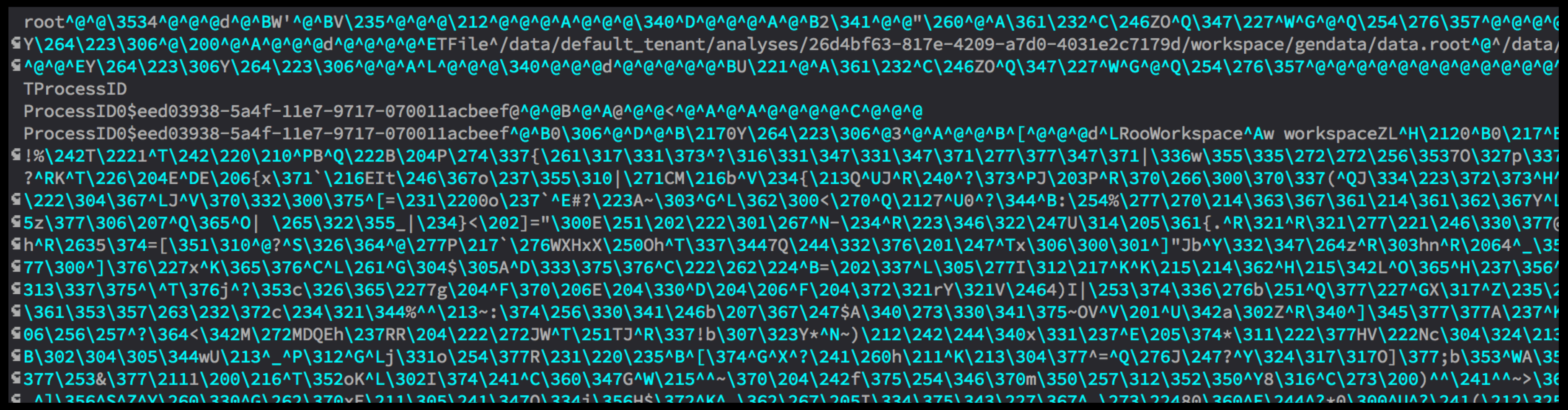


Four questions

(1) data?	✓ EOS, CephFS
(2) software?	✓ Git, SVN, local machines
(3) environment?	✓ Docker, VMs
(4) workflow?	✓ CWL, Yadage

(1) Data

- Stored on CERN Analysis Preservation
- CephFS
- EOS
- ….



```
root^@^@\3534^@^@^@d^@^BW'^@^BV\235^@^@^@\212^@^@^@^A^@^@^@\340^D^@^@^@^A^@^B2\341^@^@"\260^@^A\361\232^C\246ZO^Q\347\227^W^G^@^Q\254\276\357^@^@^@^@
Y\264\223\306^@\200^@^A^@^@^@d^@^@^@^@^ETFile^/data/default_tenant/analyses/26d4bf63-817e-4209-a7d0-4031e2c7179d/workspace/gendata/data.root^@^/data/
^@^@^EY\264\223\306Y\264\223\306^@^@^A^L^@^@^@\340^@^@^@d^@^@^@^@^@^BU\221^@^A\361\232^C\246ZO^Q\347\227^W^G^@^Q\254\276\357^@^@^@^@^@^@^@^@^@^@^
TProcessID
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ProcessID0$eed03938-5a4f-11e7-9717-070011acbeef^@^B0\306^@^D^@^B\2170Y\264\223\306^@3^@^A^@^@^B^[^@^@^@d^LRooWorkspace^Aw workspaceZL^H\2120^B0\217^E
!%\242T\2221^T\242\220\210^PB^Q\222B\204P\274\337{\261\317\331\373^?\316\331\347\331\347\371\277\377\347\371|\336w\355\335\272\272\256\3537O\327p\337
?^RK^T\226\204E^DE\206{x\371`\216EIt\246\367o\237\355\310|\271CM\216b^V\234{\213Q^UJ^R\240^?\373^PJ\203P^R\370\266\300\370\337(^QJ\334\223\372\373^H^
\222\304\367^LJ^V\370\332\300\375^[=\231\2200o\237`^E#?\223A~\303^G^L\362\300<\270^Q\2127^U0^?\344^B:\254%\277\270\214\363\367\361\214\361\362\367Y^L
5z\377\306\207^Q\365^O| \265\322\355_|\234}<\202]="\300E\251\202\222\301\267^N-\234^R\223\346\322\247U\314\205\361{.^R\321^R\321\277\221\246\330\377@
h^R\2635\374=[\351\310^@?^S\326\364^@\277P\217`\276WXHxX\250Oh^T\337\3447Q\244\332\376\201\247^Tx\306\300\301^]"Jb^Y\332\347\264z^R\303hn^R\2064^_\35
77\300^]\376\227x^K\365\376^C^L\261^G\304$\305A^D\333\375\376^C\222\262\224^B=\202\337^L\305\277I\312\217^K^K\215\214\362^H\215\342L^O\365^H\237\356^
313\337\375^\^T\376j^?\353c\326\365\2277g\204^F\370\206E\204\330^D\204\206^F\204\372\321rY\321V\2464)I|\253\374\336\276b\251^Q\377\227^GX\317^Z\235\2
\361\353\357\263\232\372c\234\321\344%^^\213~:\374\256\330\341\246b\207\367\247$A\340\273\330\341\375~OV^V\201^U\342a\302Z^R\340^]\345\377\377A\237^K
06\256\257^?\364<\342M\272MDQEh\237RR\204\222\272JW^T\251TJ^R\337!b\307\323Y*^N~)\212\242\244\340x\331\237^E\205\374*\311\222\377HV\222Nc\304\324\213
B\302\304\305\344wU\213^_^P\312^G^Lj\331o\254\377R\231\220\235^B^[\374^G^X^?\241\260h\211^K\213\304\377^=^Q\276J\247?^Y\324\317\317O]\377;b\353^WA\35
377\253&\377\2111\200\216^T\352oK^L\302I\374\241^C\360\347G^W\215^^~\370\204\242f\375\254\346\370m\350\257\312\352\350^Y8\316^C\273\200)^^\241^^~>\36
```
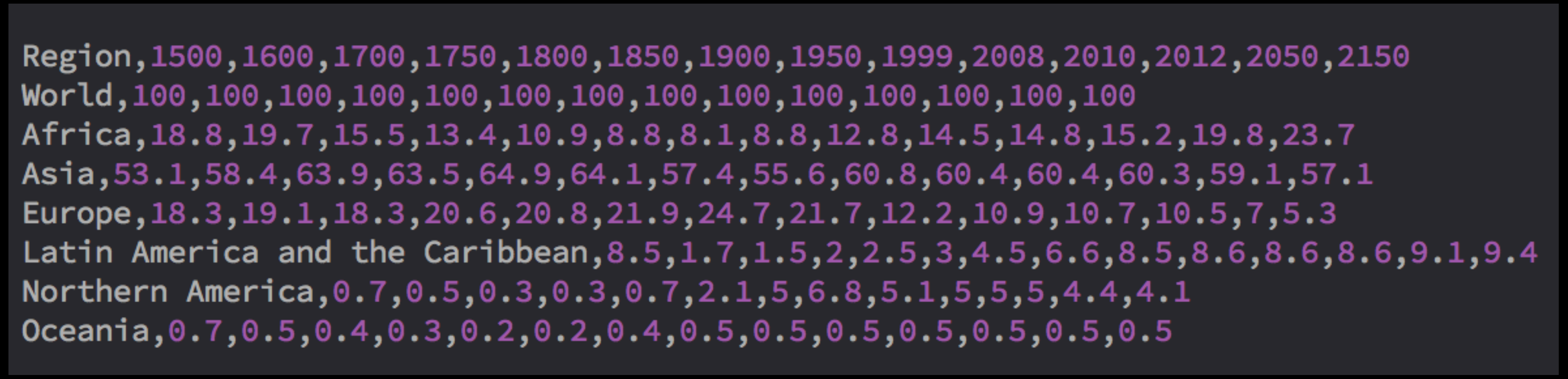

root file

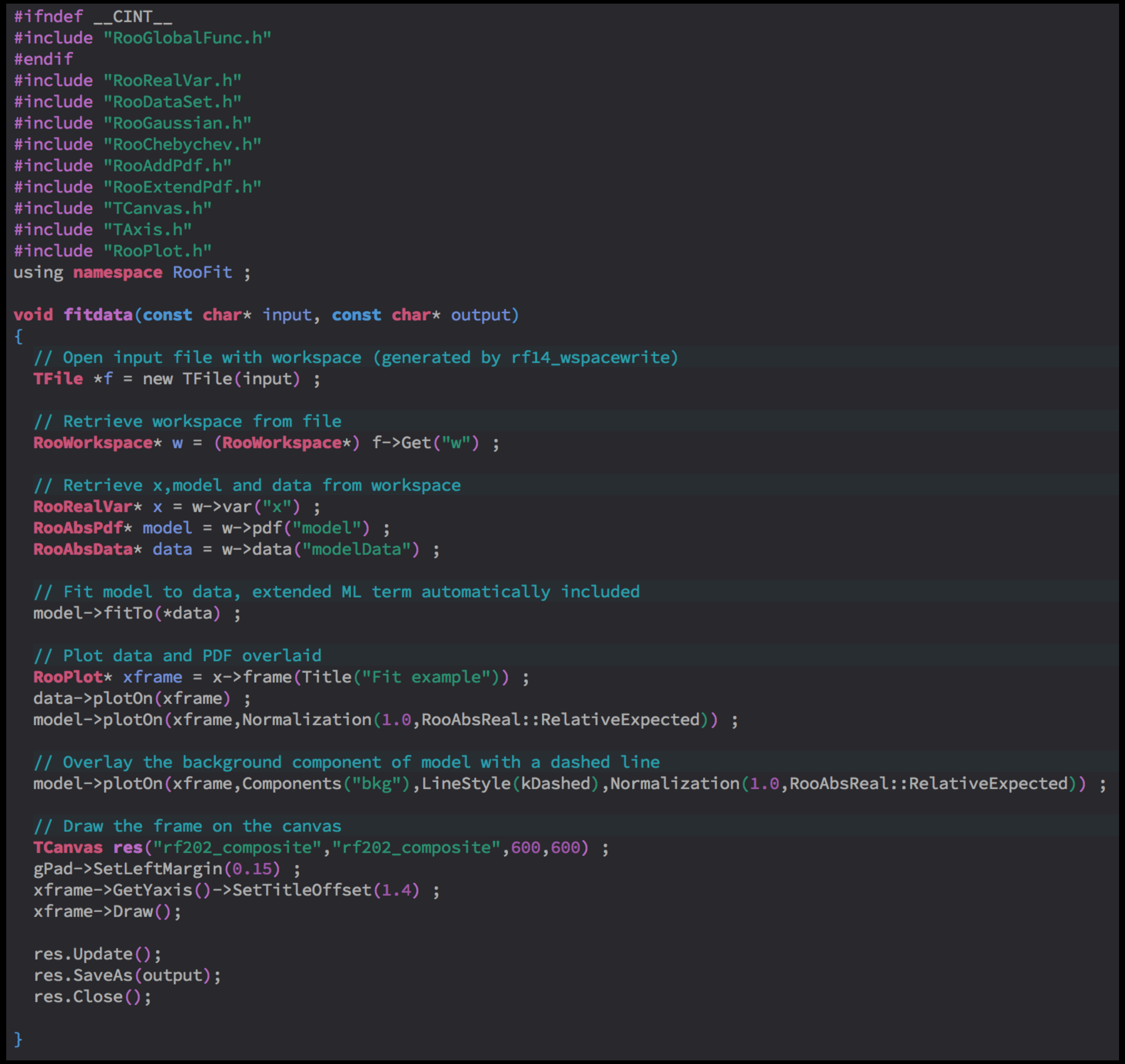


```
Region,1500,1600,1700,1750,1800,1850,1900,1950,1999,2008,2010,2012,2050,2150
World,100,100,100,100,100,100,100,100,100,100,100,100,100,100
Africa,18.8,19.7,15.5,13.4,10.9,8.8,8.1,8.8,12.8,14.5,14.8,15.2,19.8,23.7
Asia,53.1,58.4,63.9,63.5,64.9,64.1,57.4,55.6,60.8,60.4,60.4,60.3,59.1,57.1
Europe,18.3,19.1,18.3,20.6,20.8,21.9,24.7,21.7,12.2,10.9,10.7,10.5,7,5.3
Latin America and the Caribbean,8.5,1.7,1.5,2,2.5,3,4.5,6.6,8.5,8.6,8.6,8.6,9.1,9.4
Northern America,0.7,0.5,0.3,0.3,0.7,2.1,5,6.8,5.1,5,5,5,4.4,4.1
Oceania,0.7,0.5,0.4,0.3,0.2,0.2,0.4,0.5,0.5,0.5,0.5,0.5,0.5,0.5
```

CSV file

ceph EOS

(2) Software



```
#ifndef __CINT__
#include "RooGlobalFunc.h"
#endif
#include "RooRealVar.h"
#include "RooDataSet.h"
#include "RooGaussian.h"
#include "RooChebychev.h"
#include "RooAddPdf.h"
#include "RooExtendPdf.h"
#include "TCanvas.h"
#include "TAxis.h"
#include "RooPlot.h"
using namespace RooFit ;

void fitdata(const char* input, const char* output)
{
  // Open input file with workspace (generated by rf14_wspacewrite)
  TFile *f = new TFile(input) ;

  // Retrieve workspace from file
  RooWorkspace* w = (RooWorkspace*) f->Get("w") ;

  // Retrieve x,model and data from workspace
  RooRealVar* x = w->var("x") ;
  RooAbsPdf* model = w->pdf("model") ;
  RooAbsData* data = w->data("modelData") ;

  // Fit model to data, extended ML term automatically included
  model->fitTo(*data) ;

  // Plot data and PDF overlaid
  RooPlot* xframe = x->frame(Title("Fit example")) ;
  data->plotOn(xframe) ;
  model->plotOn(xframe,Normalization(1.0,RooAbsReal::RelativeExpected)) ;

  // Overlay the background component of model with a dashed line
  model->plotOn(xframe,Components("bkg"),LineStyle(kDashed),Normalization(1.0,RooAbsReal::RelativeExpected)) ;

  // Draw the frame on the canvas
  TCanvas res("rf202_composite","rf202_composite",600,600) ;
  gPad->SetLeftMargin(0.15) ;
  xframe->GetYaxis()->SetTitleOffset(1.4) ;
  xframe->Draw();

  res.Update();
  res.SaveAs(output);
  res.Close();

}
```

(3) Environment

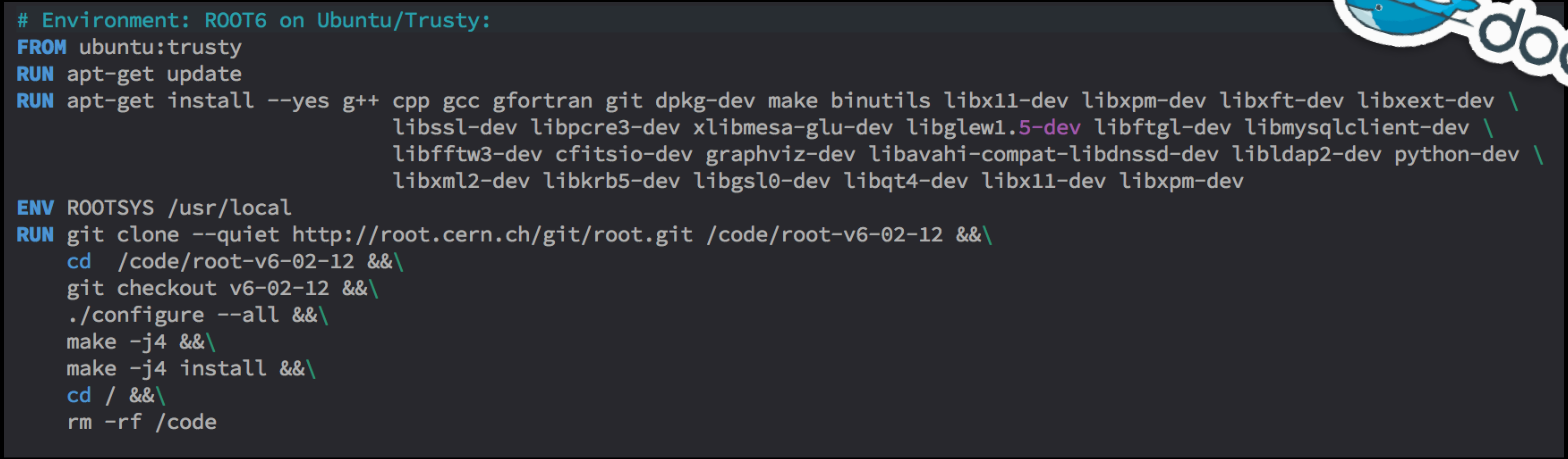
Docker support, other technologies under investigation

Encourage the usage of **base images** i.e. *reanahub/reana-env-root6* for ROOT6 analyses

Take the most out of **image layering**

Encourage **collaboration** and **reusable images**

reana-env-root6



```
# Environment: ROOT6 on Ubuntu/Trusty:
FROM ubuntu:trusty
RUN apt-get update
RUN apt-get install --yes g++ cpp gcc gfortran git dpkg-dev make binutils libx11-dev libxpm-dev libxft-dev libxext-dev \
                              libssl-dev libpcre3-dev xlibmesa-glu-dev libglew1.5-dev libftgl-dev libmysqlclient-dev \
                              libfftw3-dev cfitsio-dev graphviz-dev libavahi-compat-libdnssd-dev libldap2-dev python-dev \
                              libxml2-dev libkrb5-dev libgsl0-dev libqt4-dev libx11-dev libxpm-dev
ENV ROOTSYS /usr/local
RUN git clone --quiet http://root.cern.ch/git/root.git /code/root-v6-02-12 &&\
    cd  /code/root-v6-02-12 &&\
    git checkout v6-02-12 &&\
    ./configure --all &&\
    make -j4 &&\
    make -j4 install &&\
    cd / &&\
    rm -rf /code
```

(4) Workflow

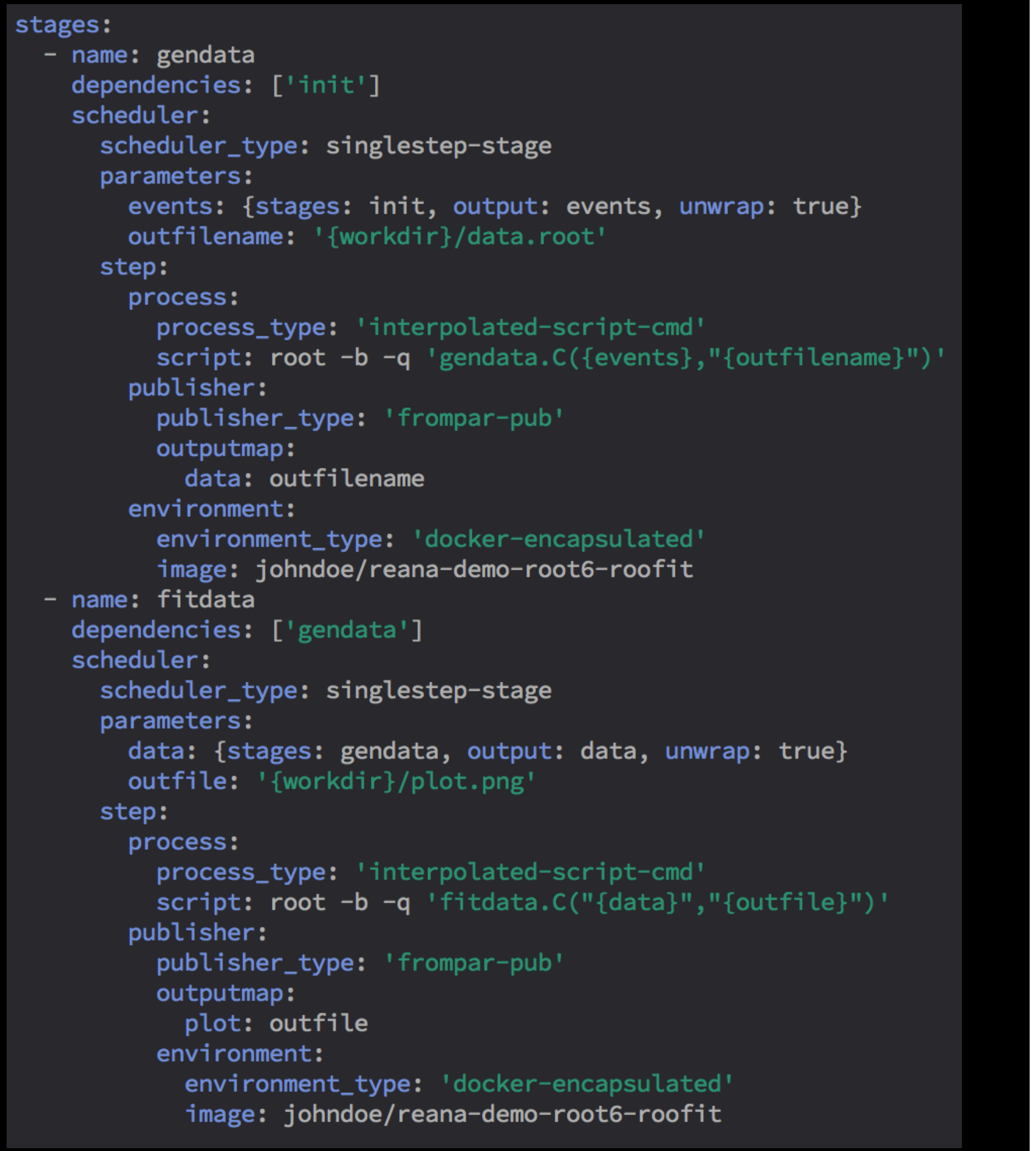
Structured computational workflows over free-text READMEs

Testable approach

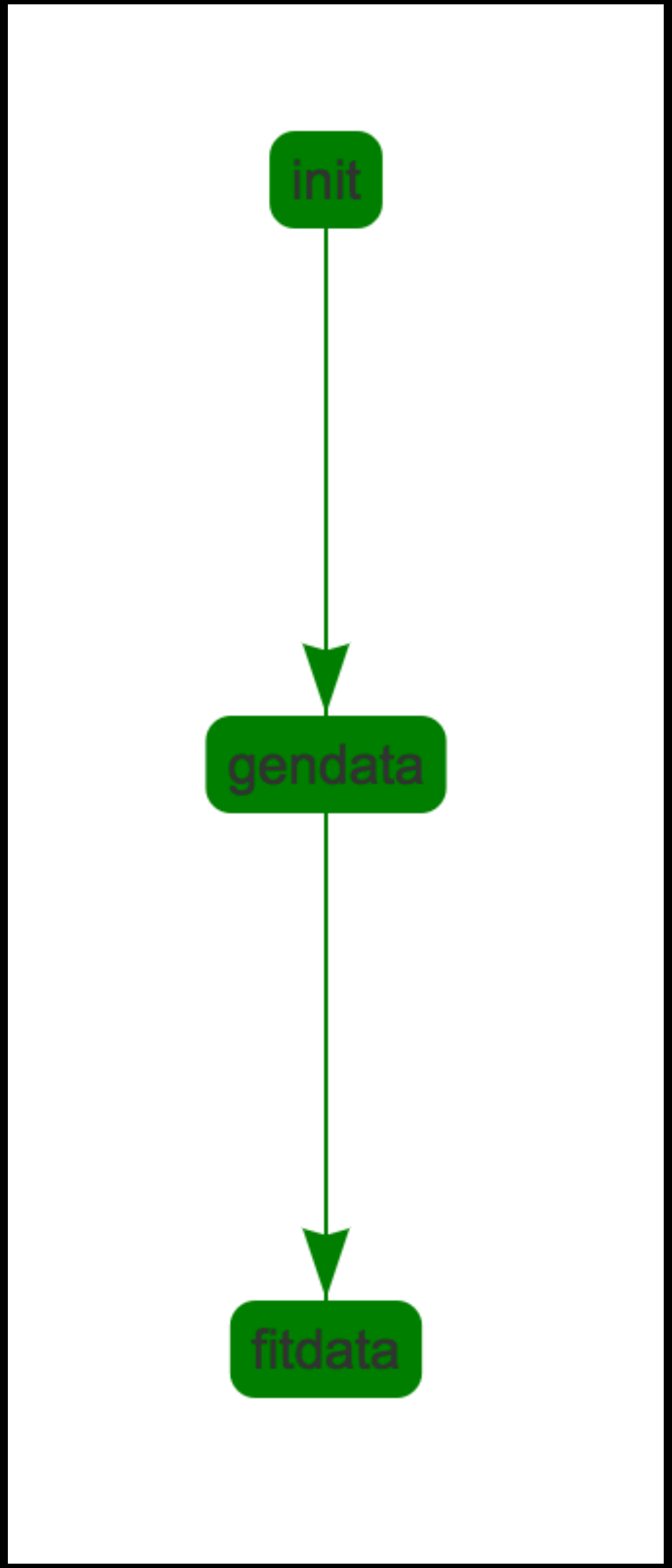
Support for Yadage workflows

Support for CWL workflows

Yadage workflow example



```
stages:
  - name: gendata
    dependencies: ['init']
    scheduler:
      scheduler_type: singlestep-stage
      parameters:
        events: {stages: init, output: events, unwrap: true}
        outfilename: '{workdir}/data.root'
      step:
        process:
          process_type: 'interpolated-script-cmd'
          script: root -b -q 'gendata.C({events},"{outfilename}")'
        publisher:
          publisher_type: 'frompar-pub'
          outputmap:
            data: outfilename
        environment:
          environment_type: 'docker-encapsulated'
          image: johndoe/reana-demo-root6-roofit
  - name: fitdata
    dependencies: ['gendata']
    scheduler:
      scheduler_type: singlestep-stage
      parameters:
        data: {stages: gendata, output: data, unwrap: true}
        outfile: '{workdir}/plot.png'
      step:
        process:
          process_type: 'interpolated-script-cmd'
          script: root -b -q 'fitdata.C("{data}","{outfile}")'
        publisher:
          publisher_type: 'frompar-pub'
          outputmap:
            plot: outfile
          environment:
            environment_type: 'docker-encapsulated'
            image: johndoe/reana-demo-root6-roofit
```

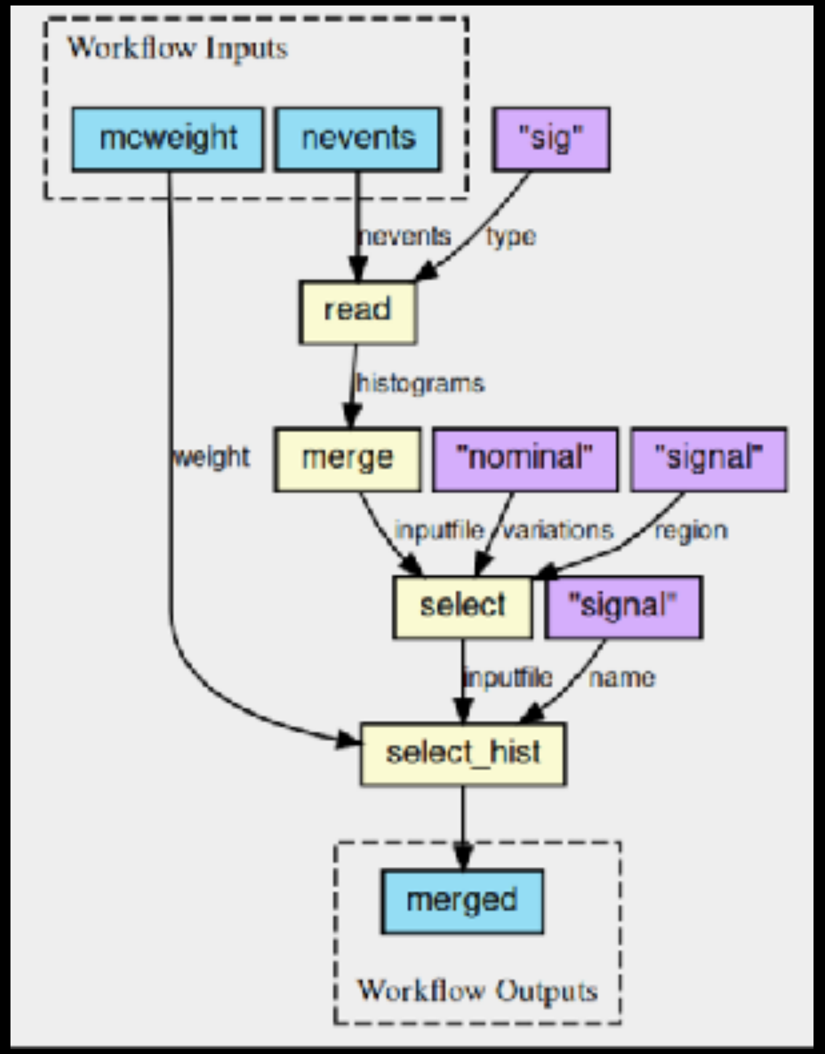


Lukas Heinrich diana-hep/yadage

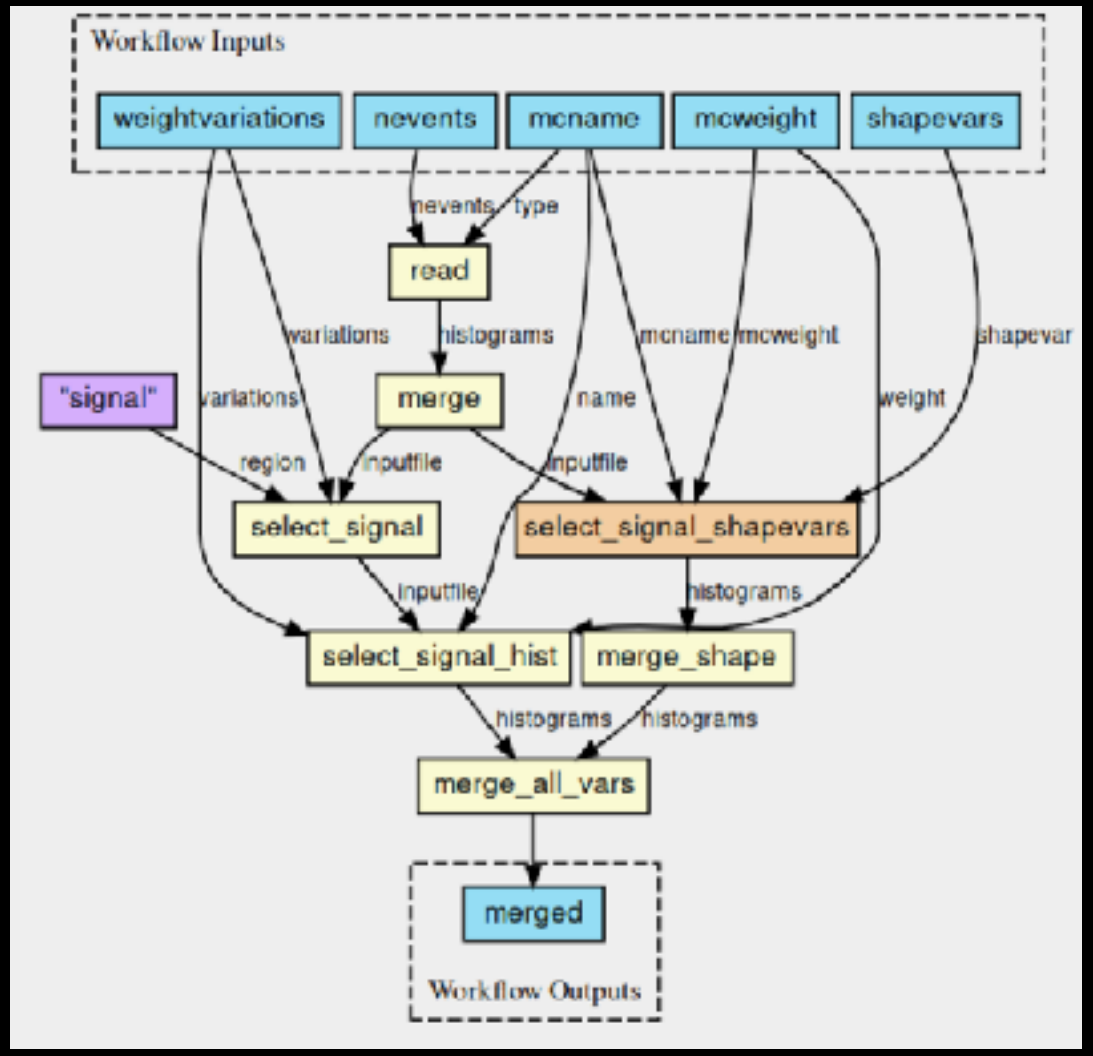
CWL workflow example

ATLAS full chain analysis example

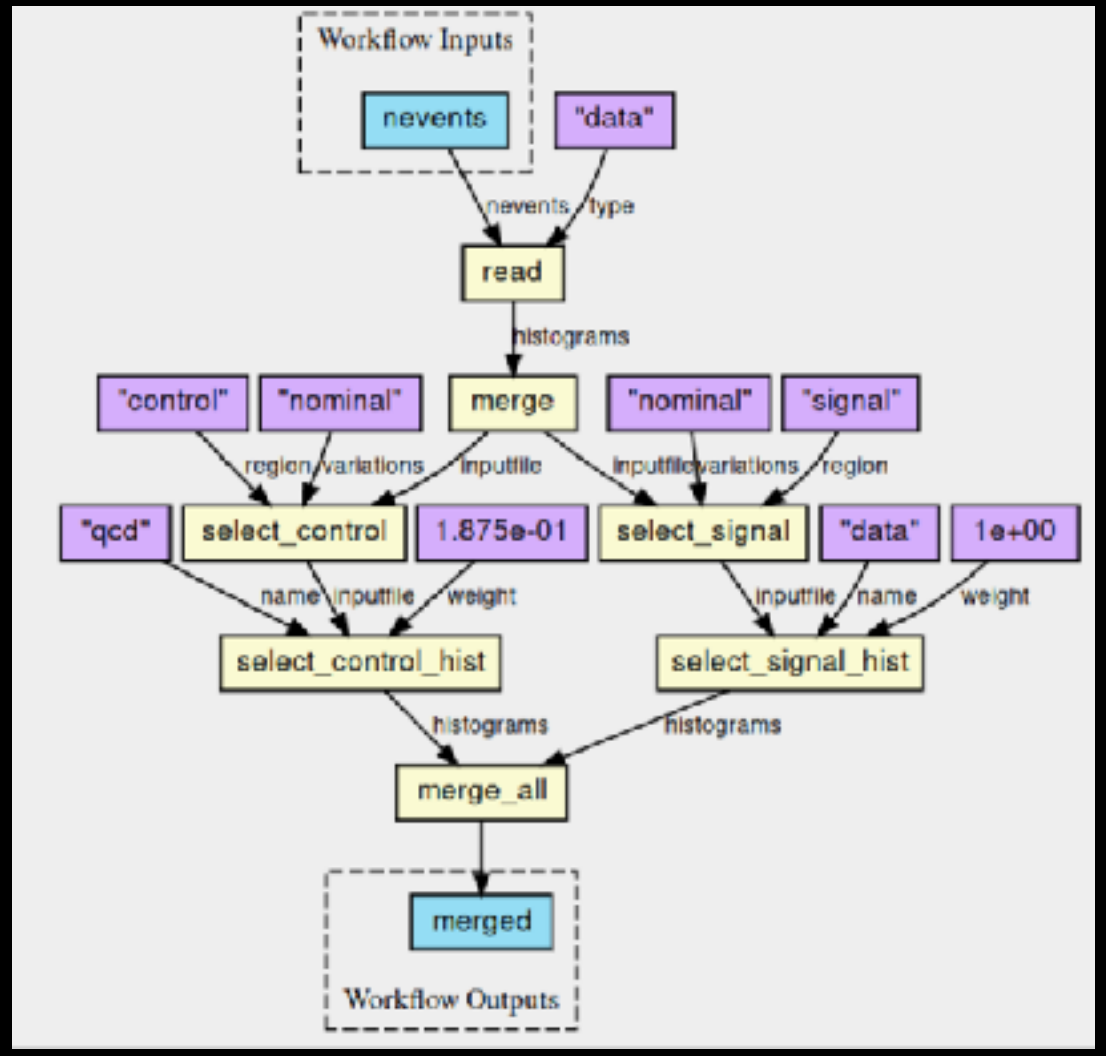
COMMON
WORKFLOW
LANGUAGE



sig



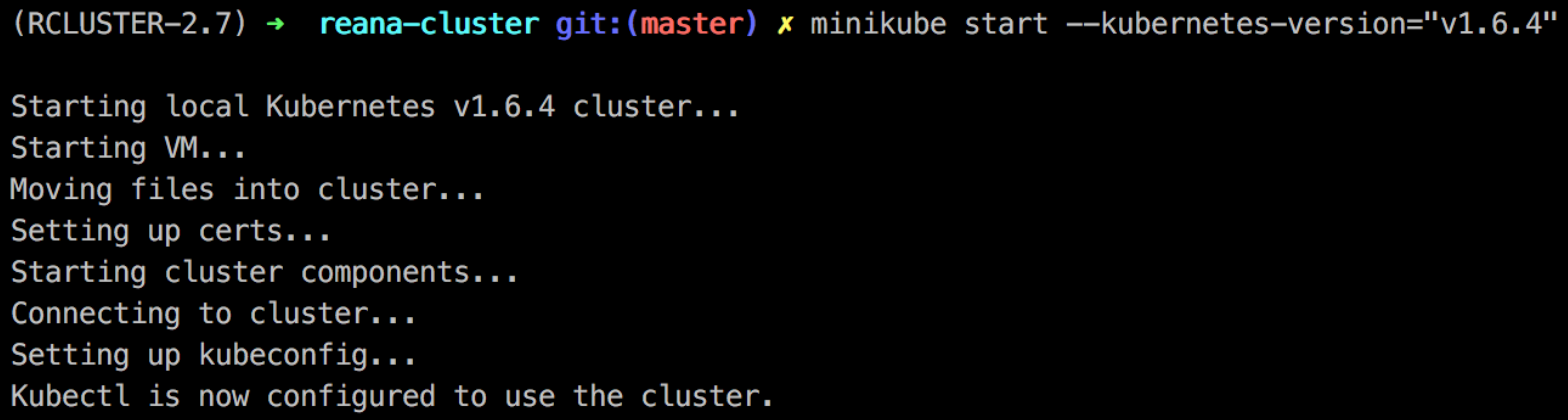
mc



data

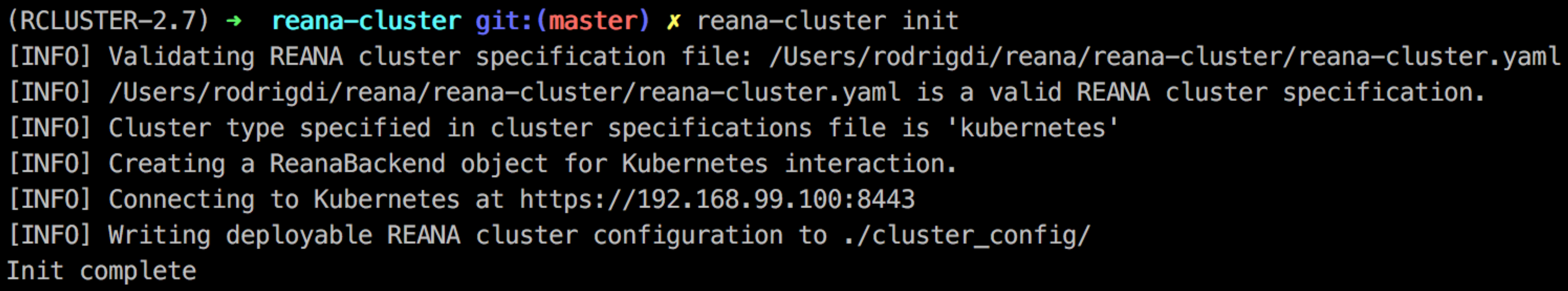
How does it work?

Deploy REANA locally



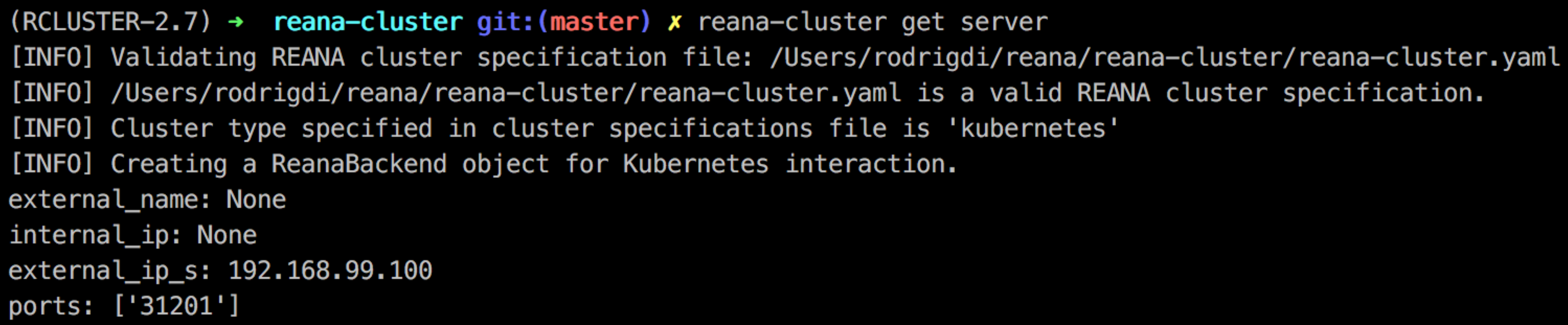
```
(RCLUSTER-2.7) ➜  reana-cluster git:(master) ✗ minikube start --kubernetes-version="v1.6.4"

Starting local Kubernetes v1.6.4 cluster...
Starting VM...
Moving files into cluster...
Setting up certs...
Starting cluster components...
Connecting to cluster...
Setting up kubeconfig...
Kubectl is now configured to use the cluster.
```

Deploy REANA locally



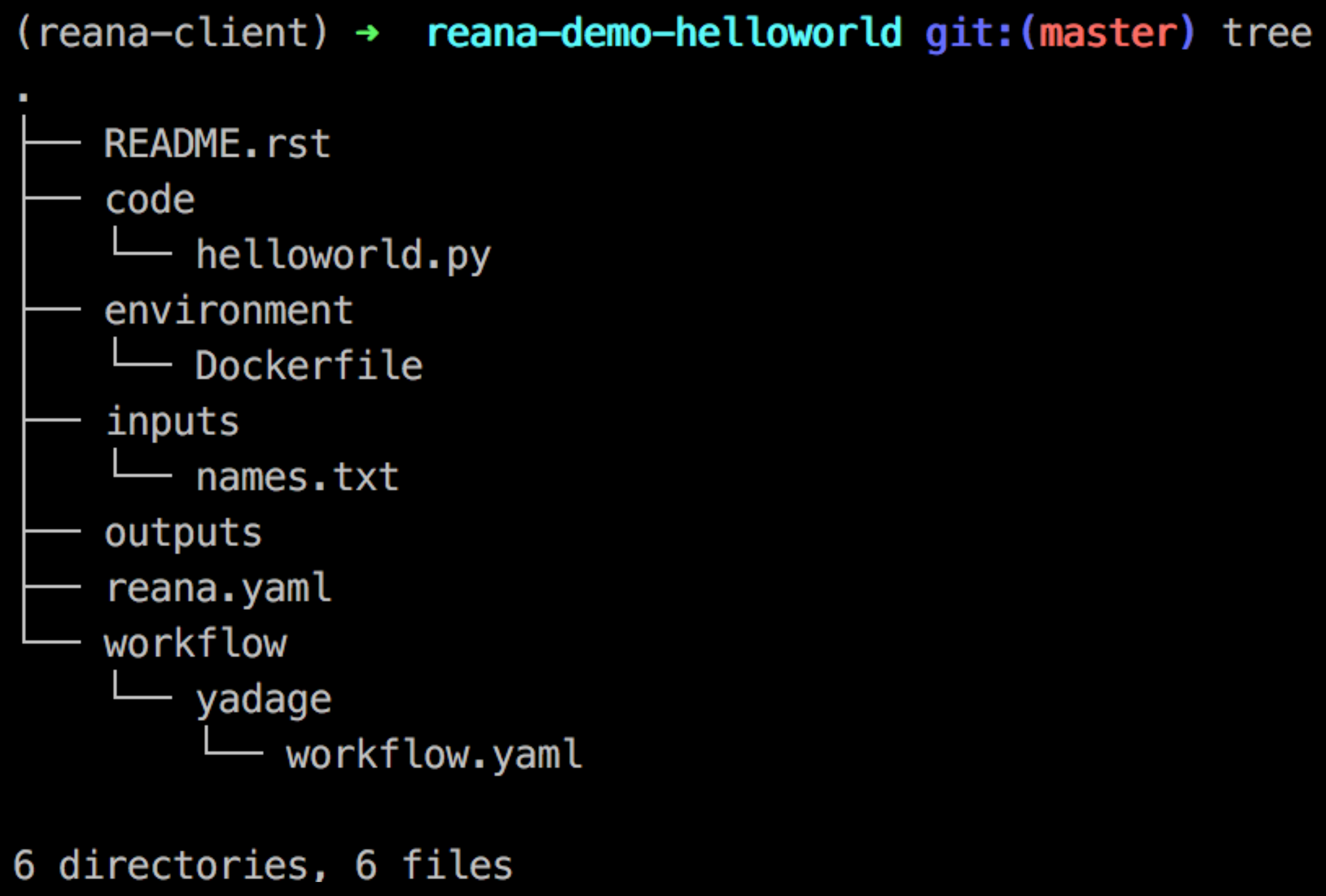
```
(RCLUSTER-2.7) ➜  reana-cluster git:(master) ✗ reana-cluster init
[INFO] Validating REANA cluster specification file: /Users/rodrigdi/reana/reana-cluster/reana-cluster.yaml
[INFO] /Users/rodrigdi/reana/reana-cluster/reana-cluster.yaml is a valid REANA cluster specification.
[INFO] Cluster type specified in cluster specifications file is 'kubernetes'
[INFO] Creating a ReanaBackend object for Kubernetes interaction.
[INFO] Connecting to Kubernetes at https://192.168.99.100:8443
[INFO] Writing deployable REANA cluster configuration to ./cluster_config/
Init complete
```

Deploy REANA locally



```
(RCLUSTER-2.7) ➜  reana-cluster git:(master) ✗ reana-cluster get server
[INFO] Validating REANA cluster specification file: /Users/rodrigdi/reana/reana-cluster/reana-cluster.yaml
[INFO] /Users/rodrigdi/reana/reana-cluster/reana-cluster.yaml is a valid REANA cluster specification.
[INFO] Cluster type specified in cluster specifications file is 'kubernetes'
[INFO] Creating a ReanaBackend object for Kubernetes interaction.
external_name: None
internal_ip: None
external_ip_s: 192.168.99.100
ports: ['31201']
```

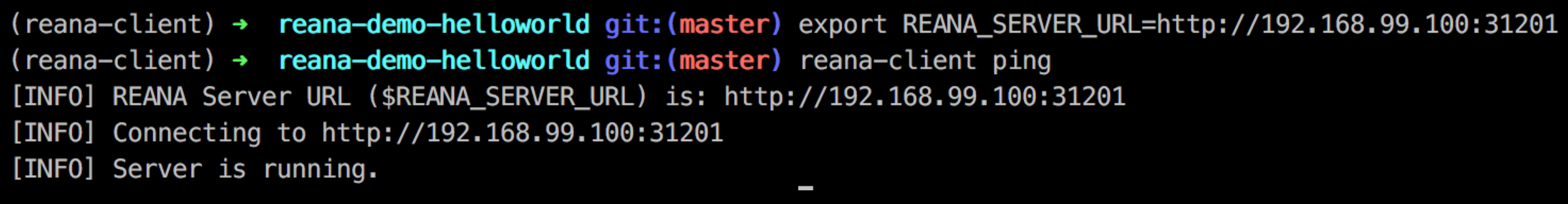
Example analysis



```
(reana-client) ➜  reana-demo-helloworld git:(master) tree
.
├── README.rst
├── code
│   └── helloworld.py
├── environment
│   └── Dockerfile
├── inputs
│   └── names.txt
├── outputs
├── reana.yaml
└── workflow
    └── yadage
        └── workflow.yaml

6 directories, 6 files
```

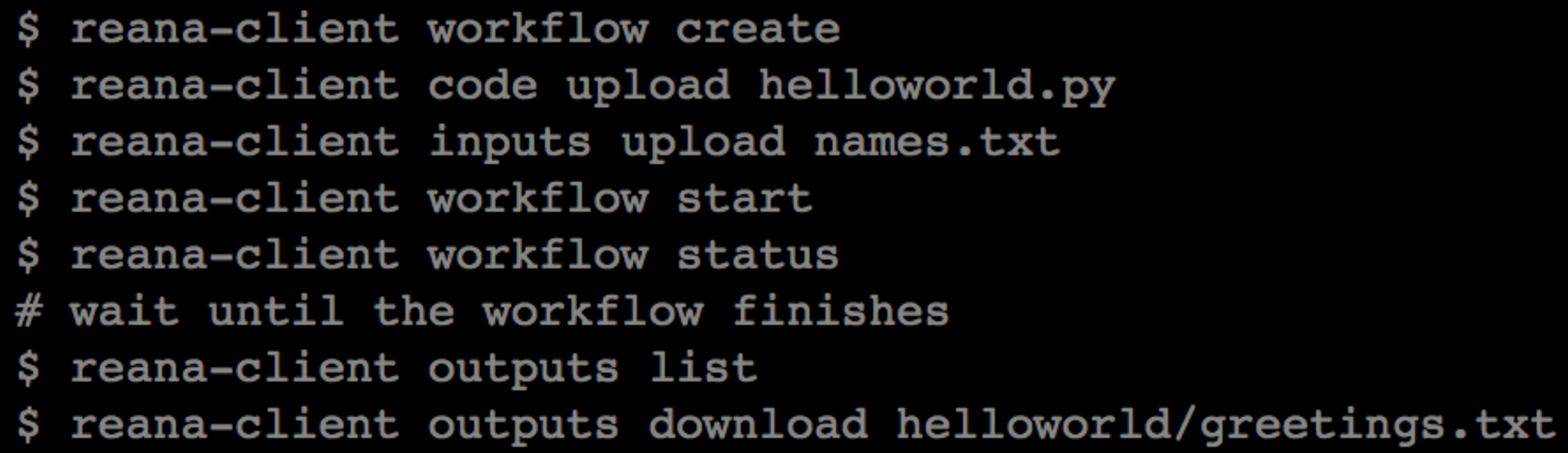
Available at https://github.com/reanahub/reana-demo-helloworld

Run on REANA



```
(reana-client) ➜  reana-demo-helloworld git:(master) export REANA_SERVER_URL=http://192.168.99.100:31201
(reana-client) ➜  reana-demo-helloworld git:(master) reana-client ping
[INFO] REANA Server URL ($REANA_SERVER_URL) is: http://192.168.99.100:31201
[INFO] Connecting to http://192.168.99.100:31201
[INFO] Server is running.
```

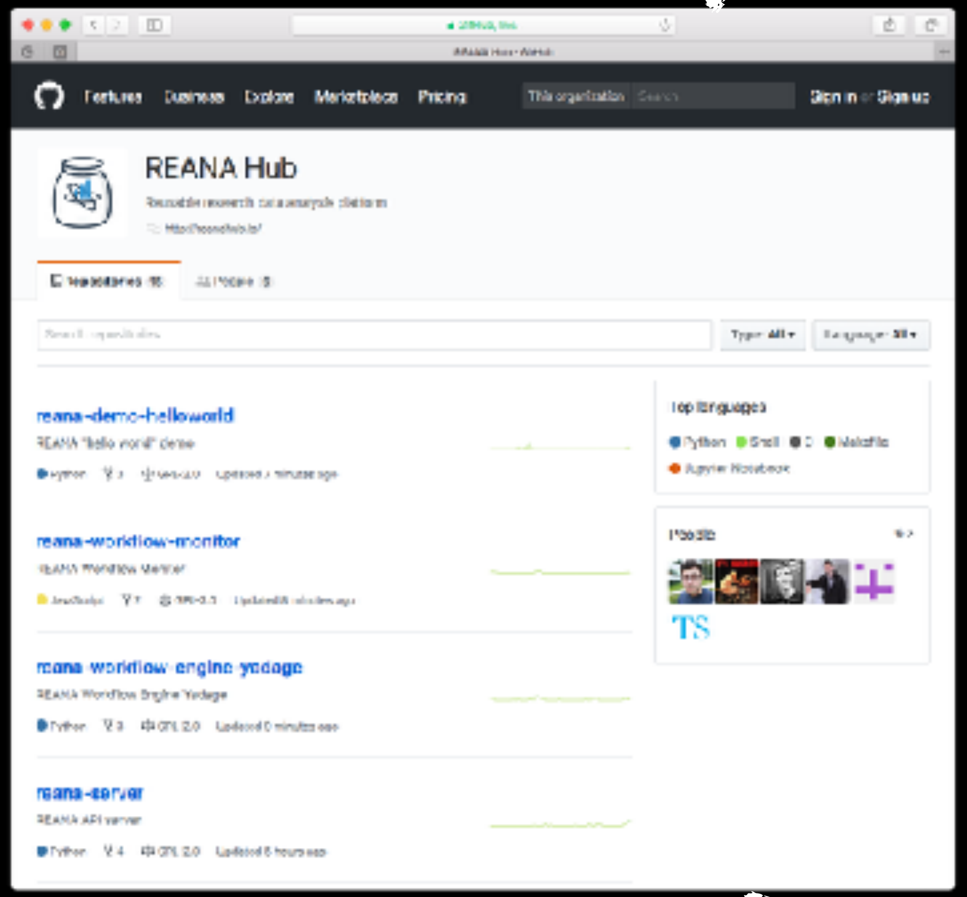
Run on REANA



```
$ reana-client workflow create
$ reana-client code upload helloworld.py
$ reana-client inputs upload names.txt
$ reana-client workflow start
$ reana-client workflow status
# wait until the workflow finishes
$ reana-client outputs list
$ reana-client outputs download helloworld/greetings.txt
```

Reusability Preservation

preserve



REANA Hub

Reusable research data analysis platform

http://reanahub.io/

reana-demo-helloworld

REANA "Hello world" demo

● Python

reana-workflow-monitor

REANA Workflow Monitor

● JavaScript

reana-workflow-engine-yadage

REANA Workflow Engine Yadage

● Python 3 GPL 2.0 Updated 0 minutes ago

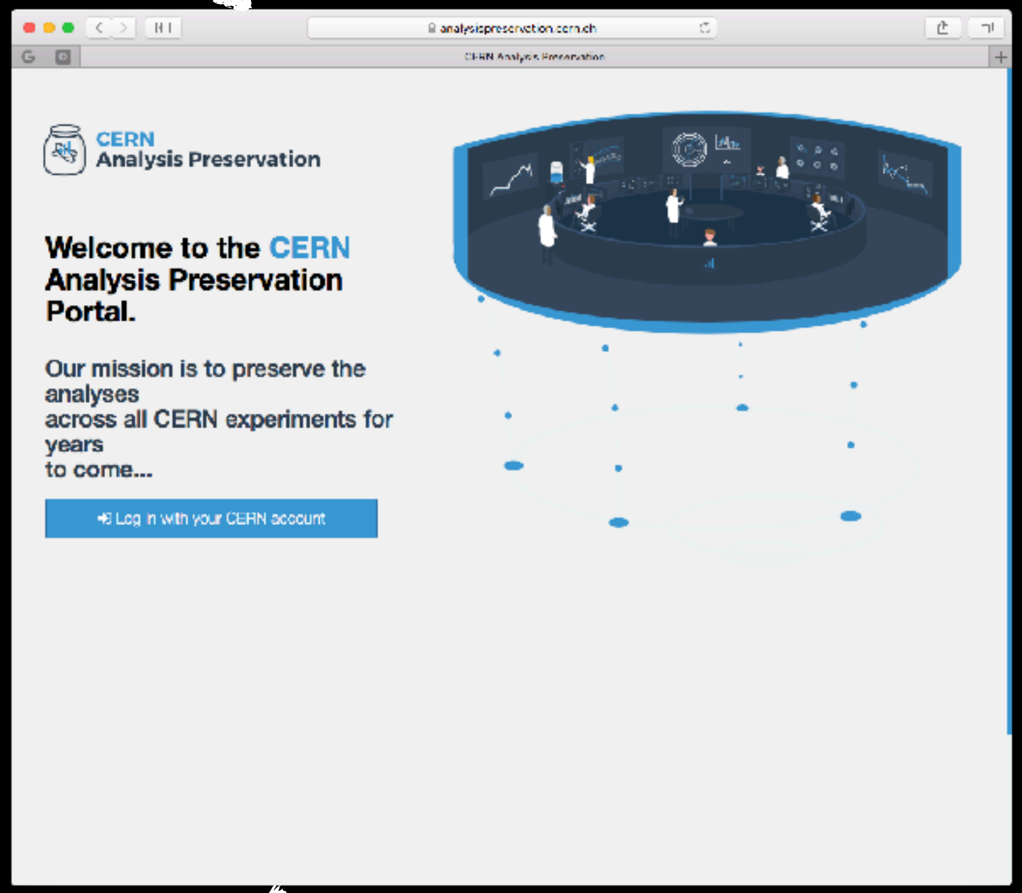
reana-server

REANA API server

● Python 4 GPL 2.0 Updated 6 hours ago

use

archive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Analysis Preservation

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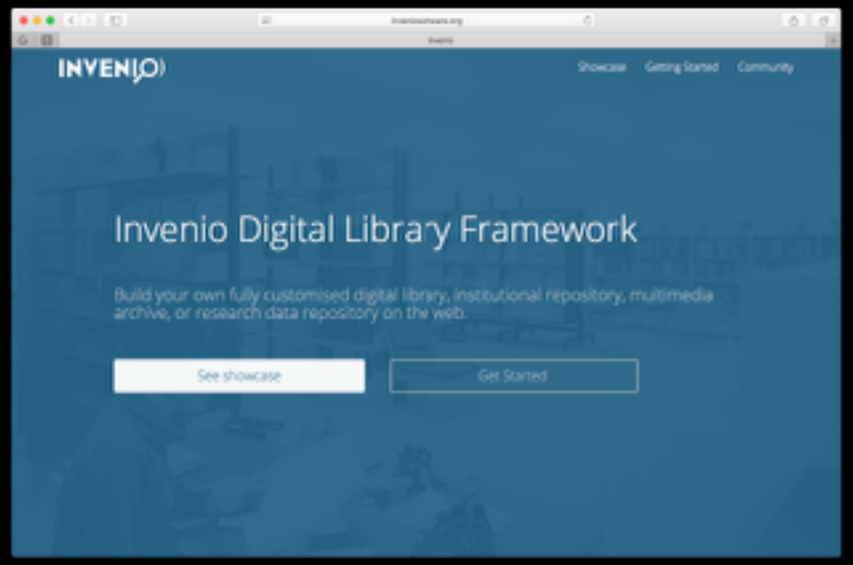
Our mission is to preserve the
analyses
across all CERN experiments for
years
to come...

Log in with your CERN account

reuse

Challenges

Social	adopting structured computational workflow specifications
	publish or perish culture
	scientific benefit vs cost of preservation
Data	Ever-increasing data size?
Software	Ever-changing computing technology?



Invenio Digital Library Framework

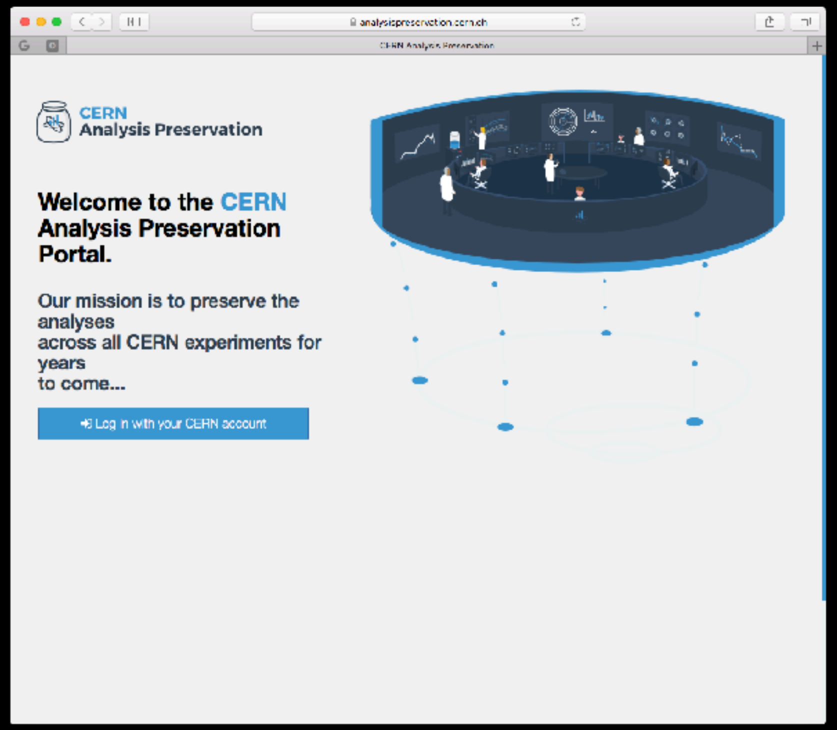
Build your own fully customised digital library, institutional repository, multimedia archive, or research data repository on the web.

http://inveniosoftware.org

http://github.com/inveniosoftware

@inveniosoftware

info@inveniosoftware.org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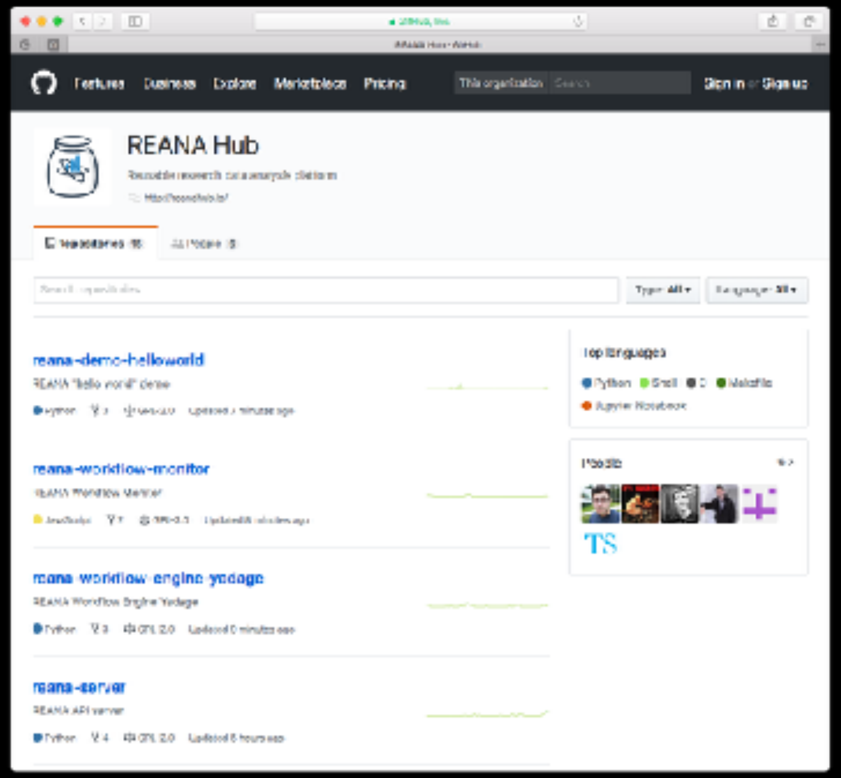
http://analysispreservation.cern.ch

http://github.com/cernanalysispreservation

analysis-preservation-support@cern.ch



REANA Hub

Reusable research data analysis platform

reana-demo-helloworld

REANA "hello world" demo

reana-workflow-monitor

REANA Workflow Monitor

reana-workflow-engine-yadage

REANA Workflow Engine Yadage

reana-server

REANA API server

http://reanahub.io

http://github.com/reanahub

@reanahub

info@reanahub.io

Questions?