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Leveraging distributed resources through high throughput analysis platforms for enhancing HEP data analyses

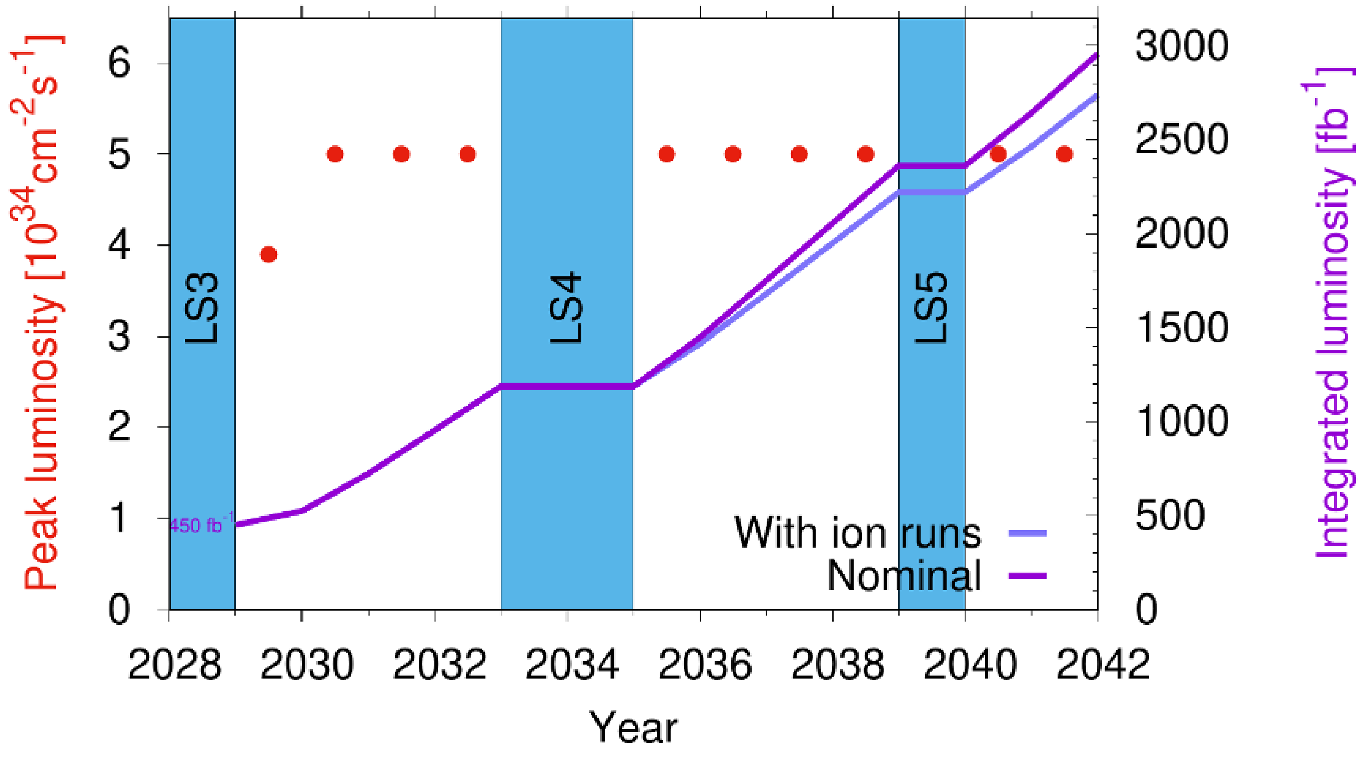
Adelina D'Onofrio[1], Tommaso Diotalevi[1,3], Francesco Giuseppe Gravili[1,5], Salvatore Loffredo[1,2], Elvira Rossi[1,2], Federica Maria Simone[1,4], Bernardino Spisso[1]
on behalf of the ATLAS and CMS Collaborations

1 INFN, 2 University Federico II, 3 University of Bologna, 4 Polytechnic Bari, 5 Università del Salento

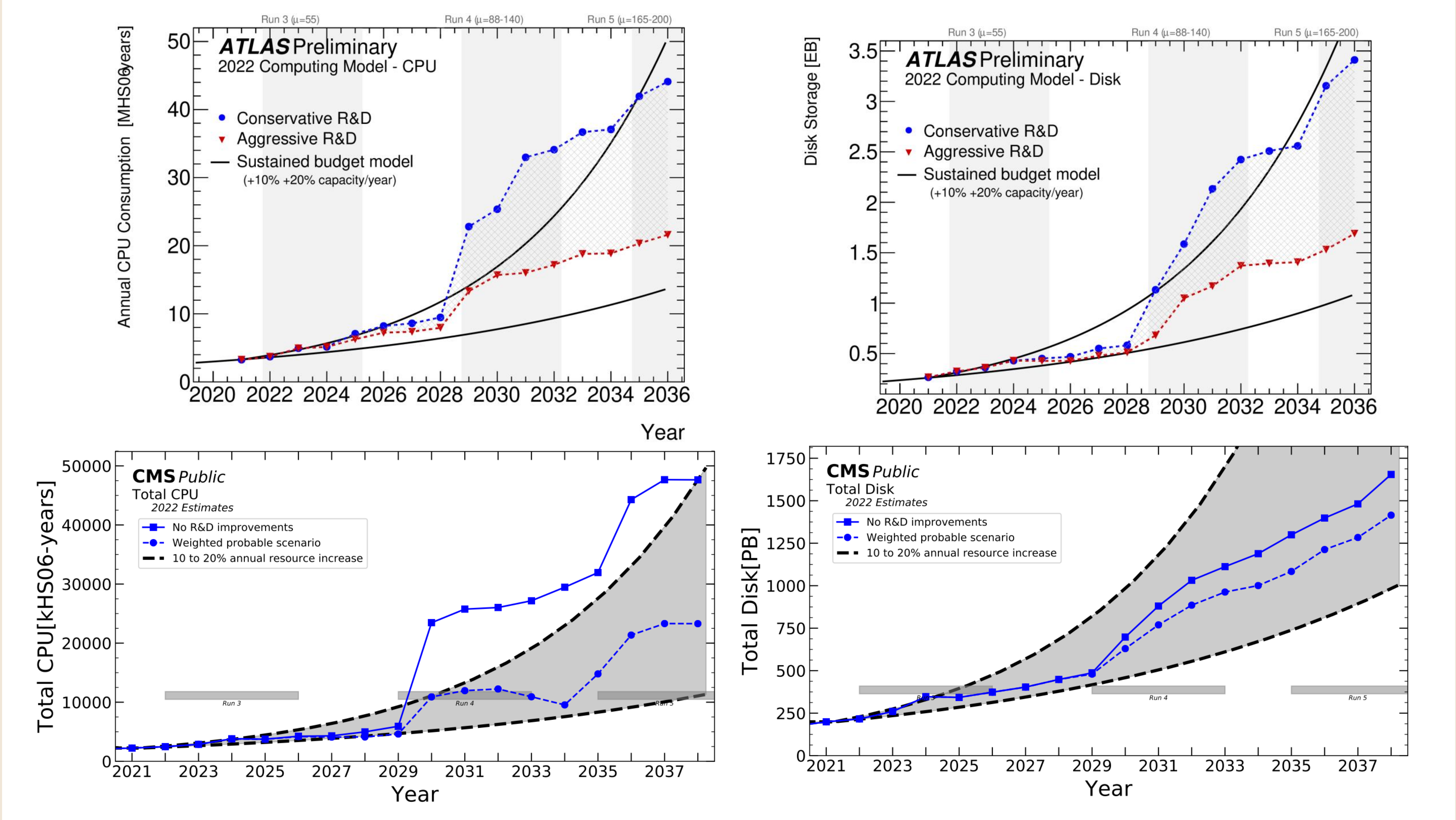
~~CHEP2024, 19-25 Oct 2024, Krakow~~ → ROOT PPP

Motivations

- **Challenges of LHC, and HL-LHC** are pushing to **re-think the HEP computing models**
  - Impact on several aspects, from software to the computing infrastructure



Similar trends for ATLAS and CMS HL-LHC projections



Higher rates of collision events → **Higher demand for computing and storage resources**

Need to:

- Optimize the usage of CPU and storage
- Promote the usage of better data formats
- **Develop new analysis paradigms**!
- New software based on declarative programming and interactive workflows
- Distribute on geographically separated resources

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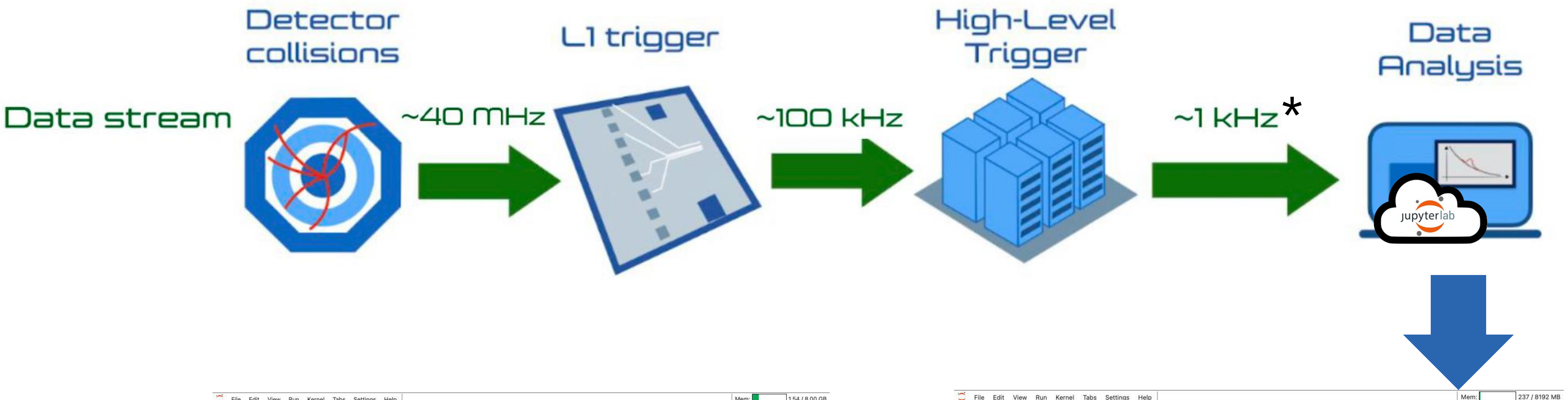
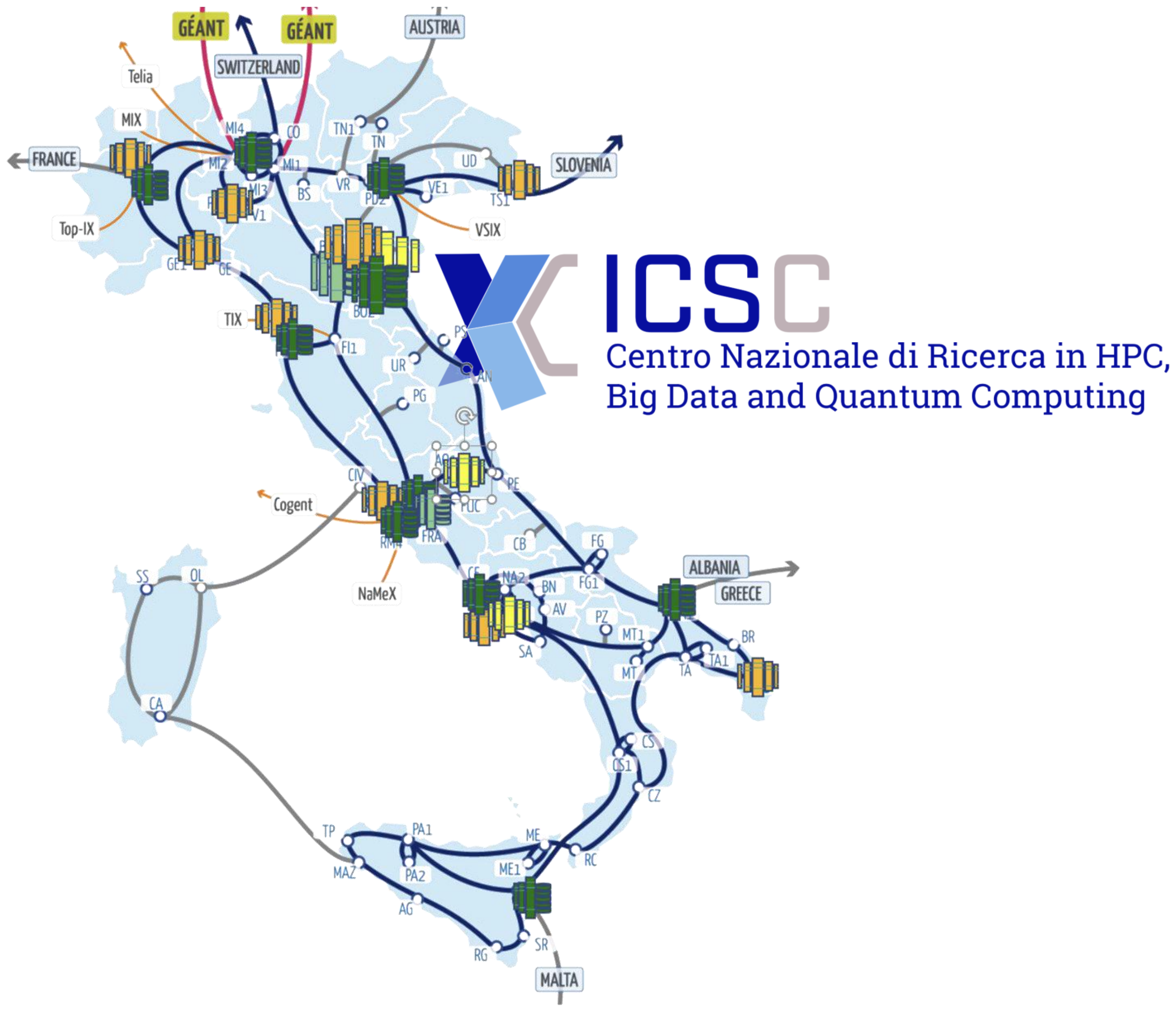
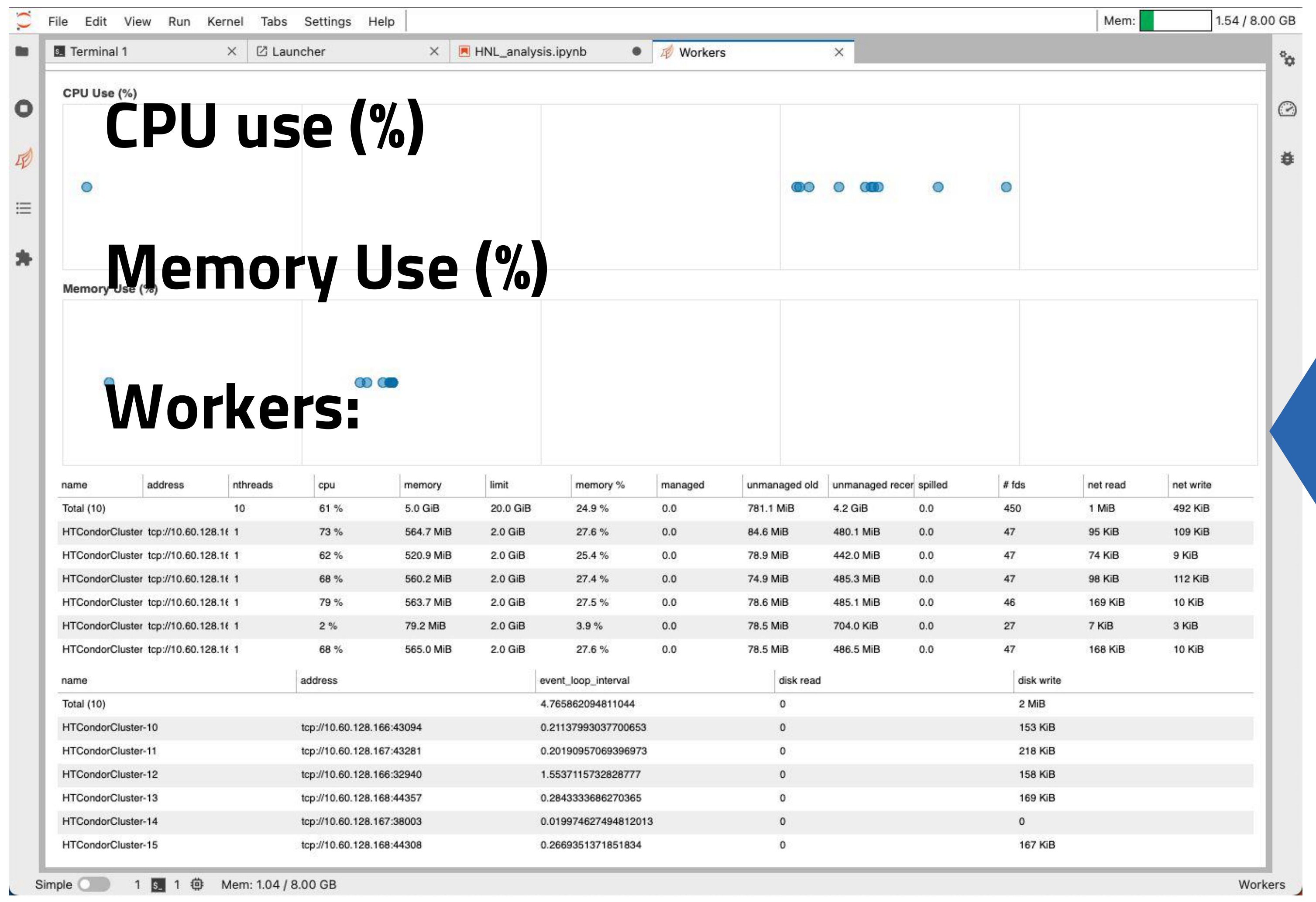
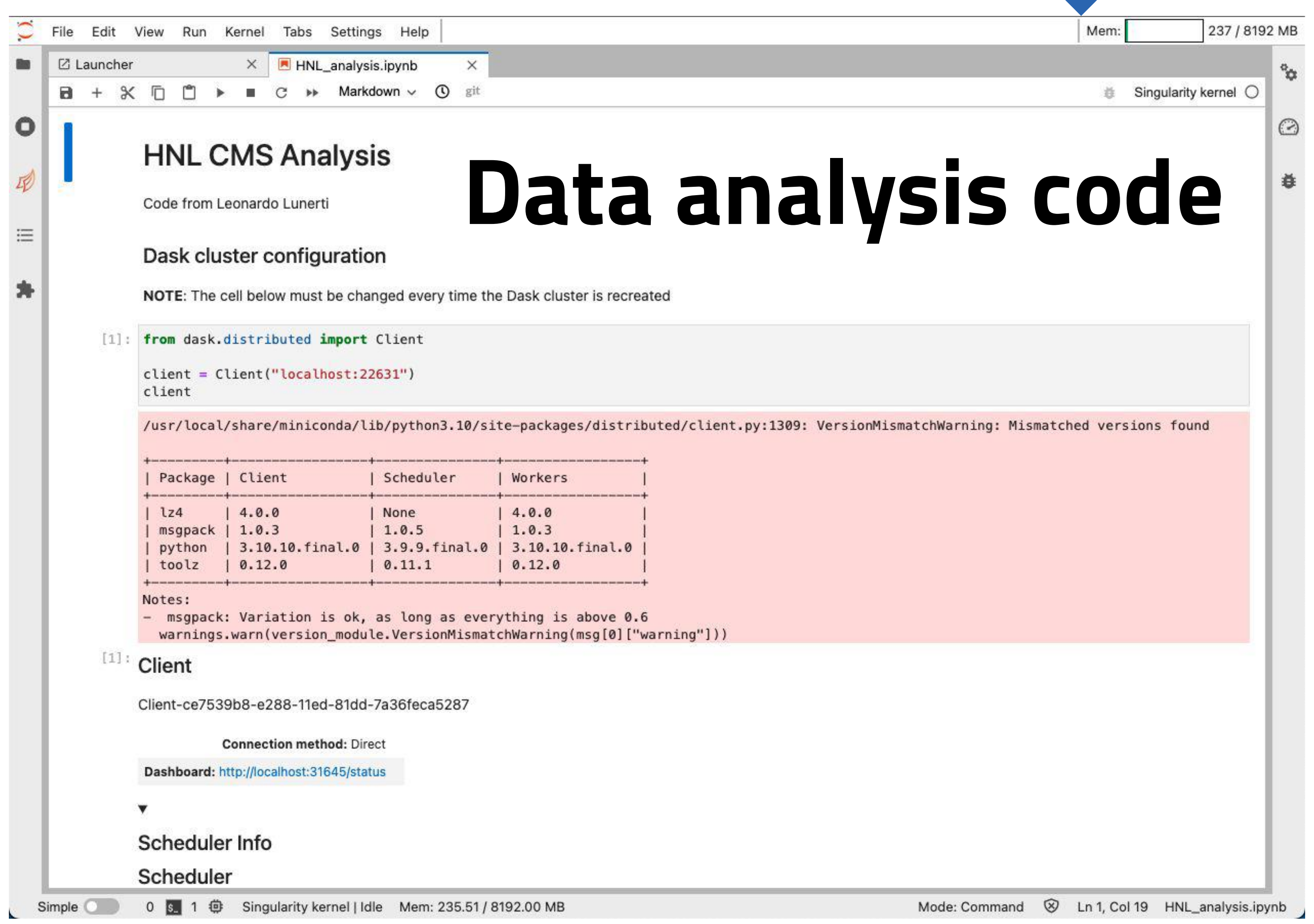
HEP data analysis with ICSC







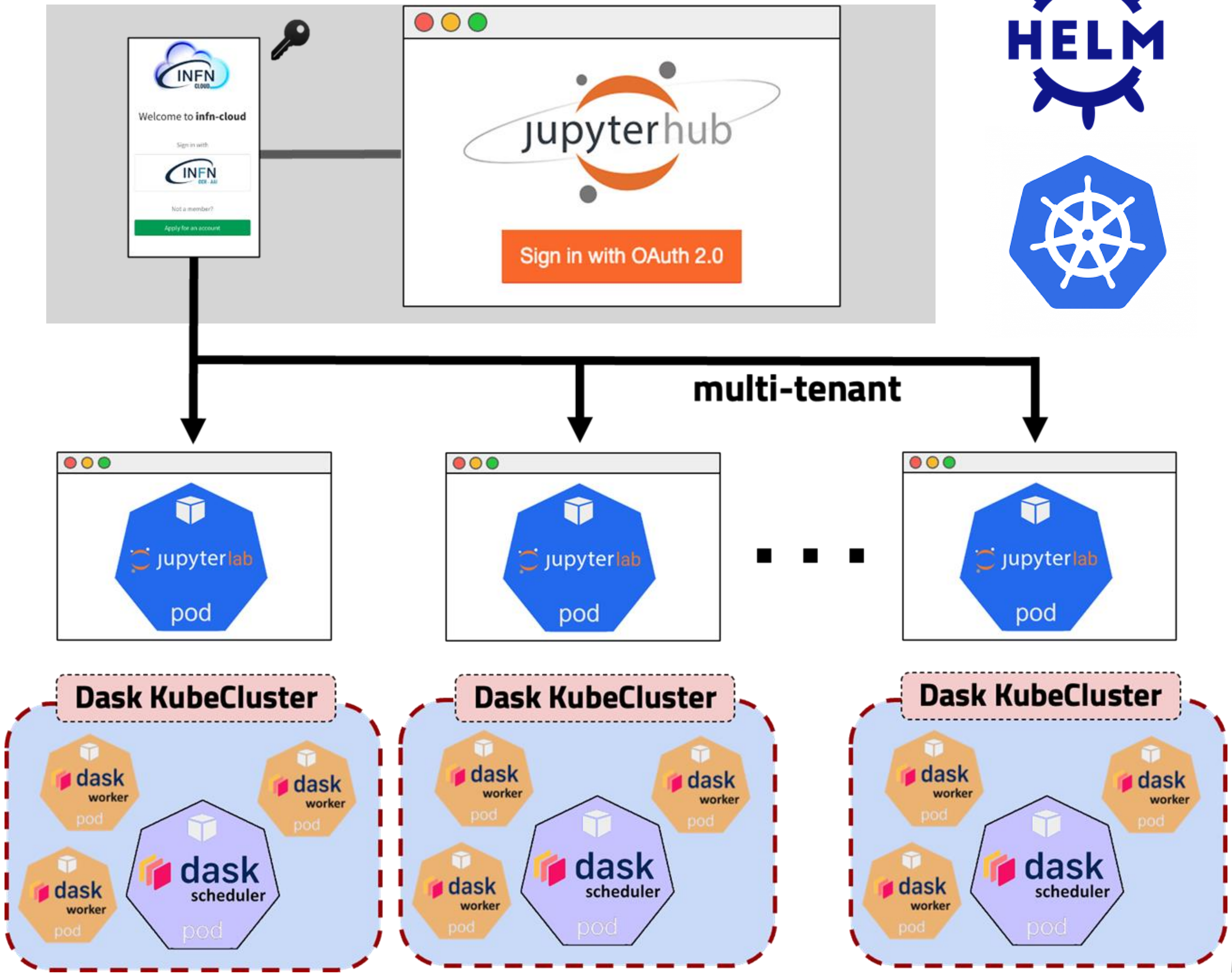


*trigger rates for previous Runs, now factor 3 ÷ 5 higher, will further scale in HL-LHC

High throughput data analysis platform

- After connecting to an entrypoint URL, the user reaches a Jupyterhub instance that, after authentication and authorization via INDIGO-IAM, allocates the required resources for the user's working area.

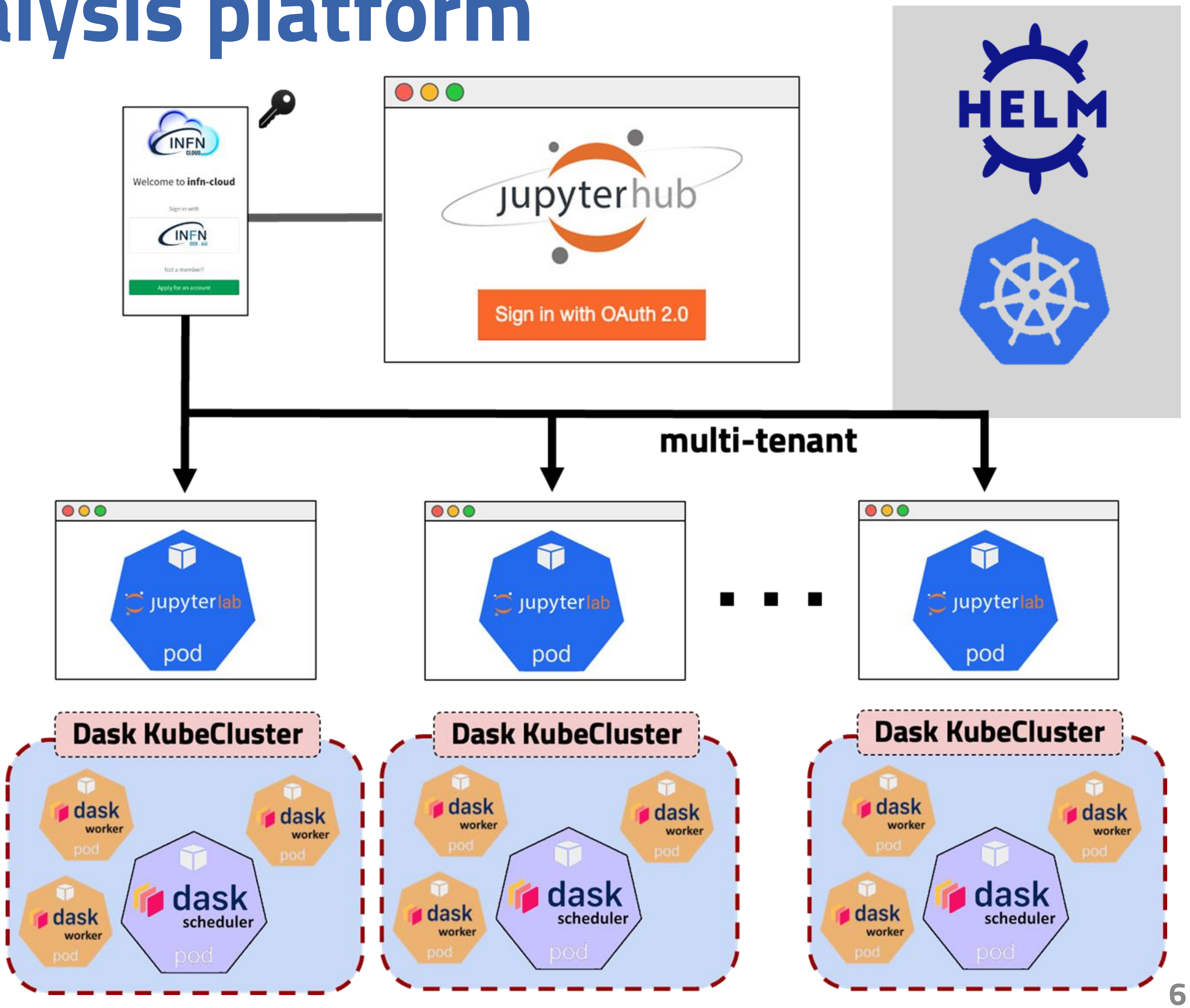
- The jupyterhub is deployed on a Kubernetes (k8s) cluster with **128 vCPUs and 258 GB**, divided into 8 nodes configured via RKE2



High throughput data analysis platform

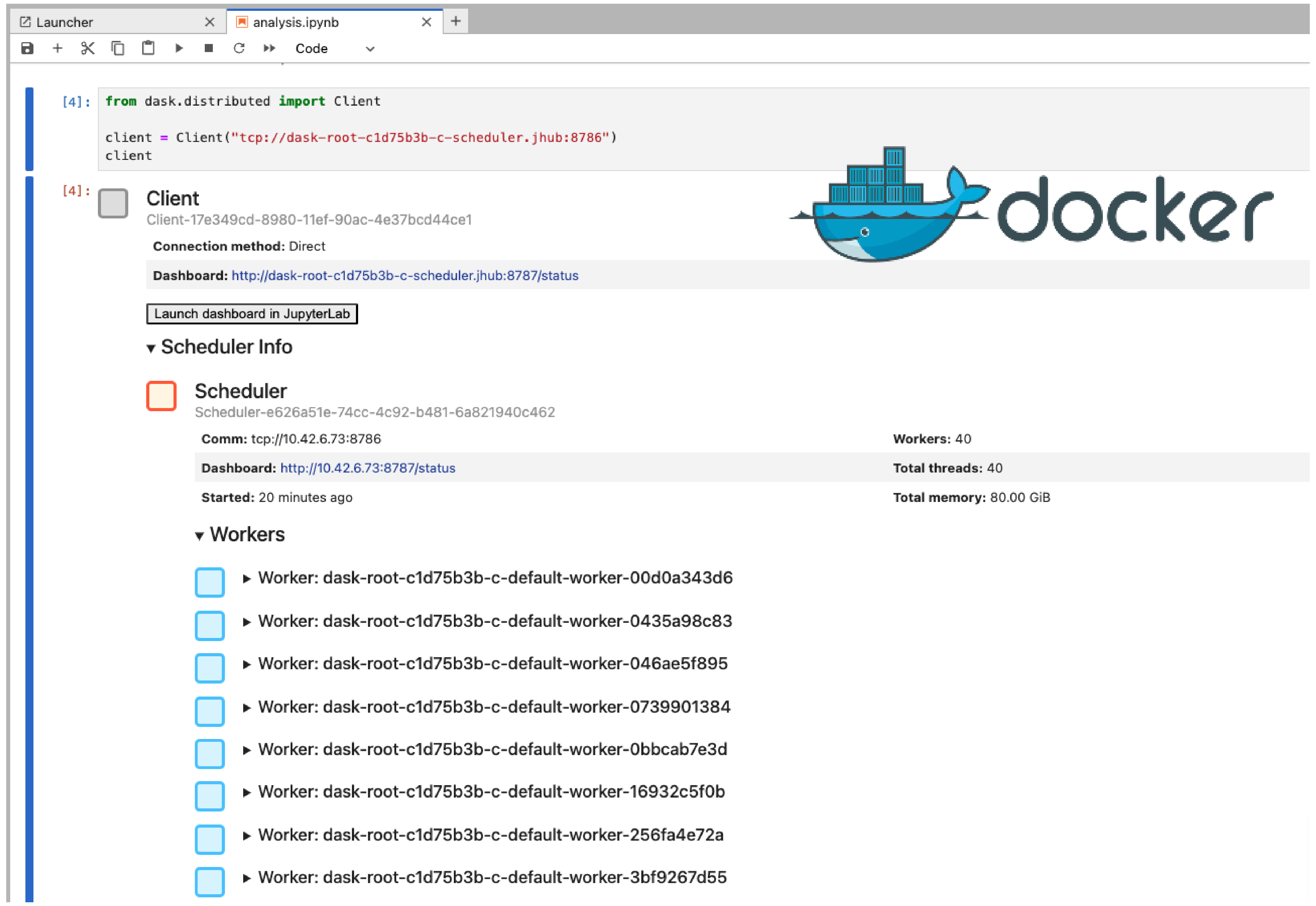
- The deployment of the Kubernetes resources is handled via HELM charts in the official Spoke2 Jhub HELM repo

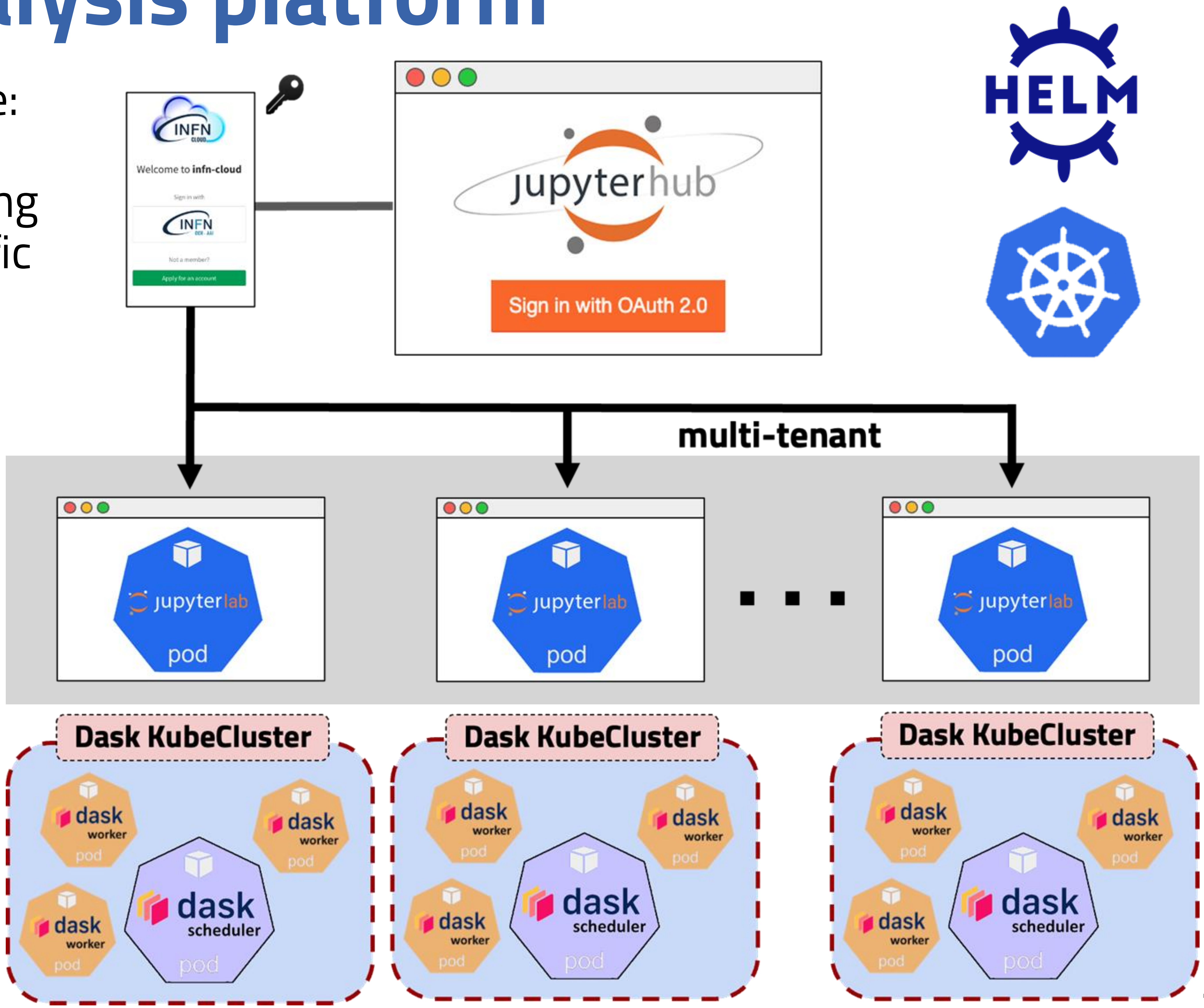
- This allows for a scalable and fault-tolerant deployment of the available resources



High throughput data analysis platform

- Jupyterlab interface is flexible and customizable:
  - Includes specific plugins (e.g. Dask)
  - Working environment highly customizable using Docker containers allowing for experiment specific software





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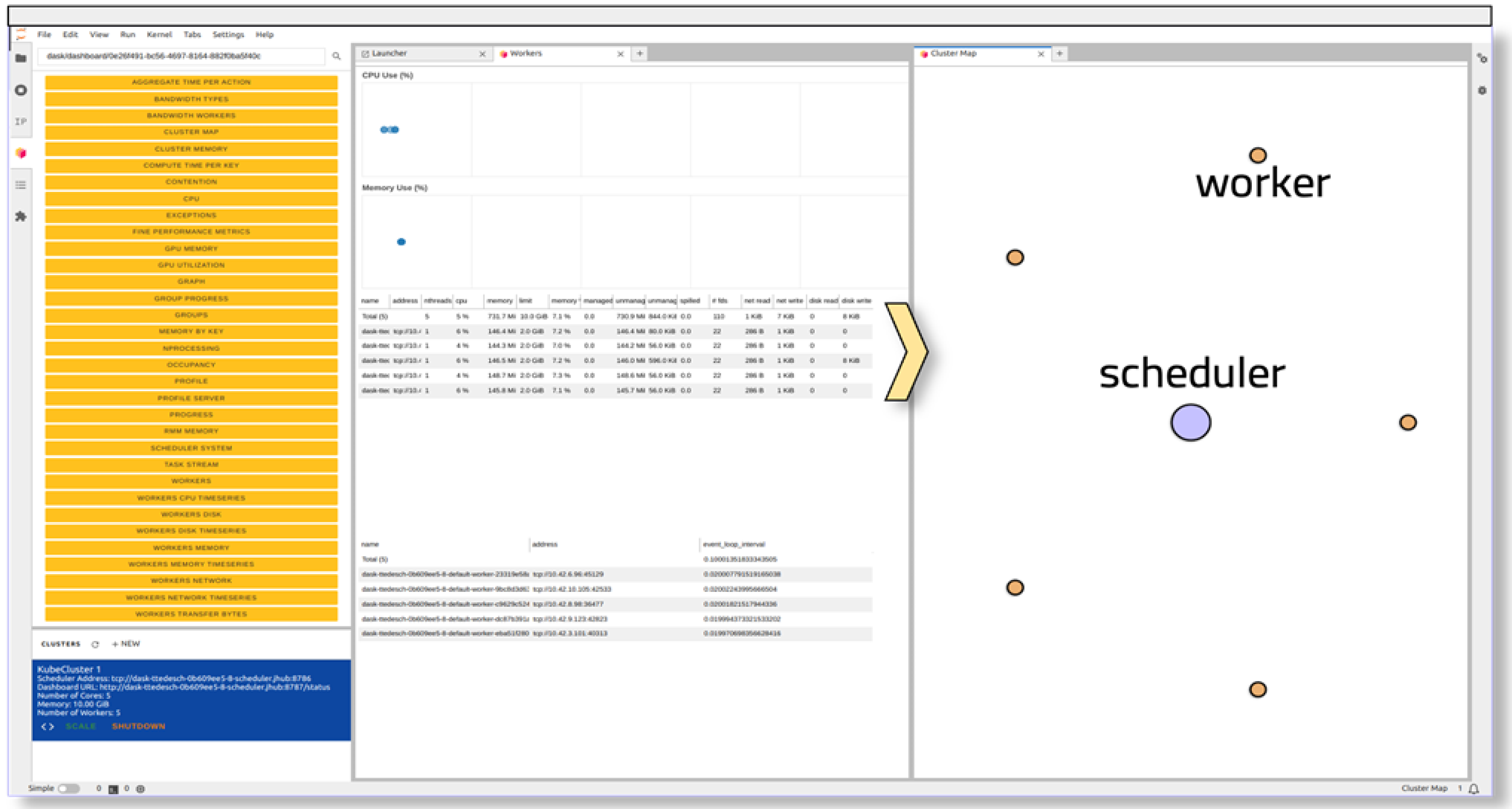
High throughput data analysis platform

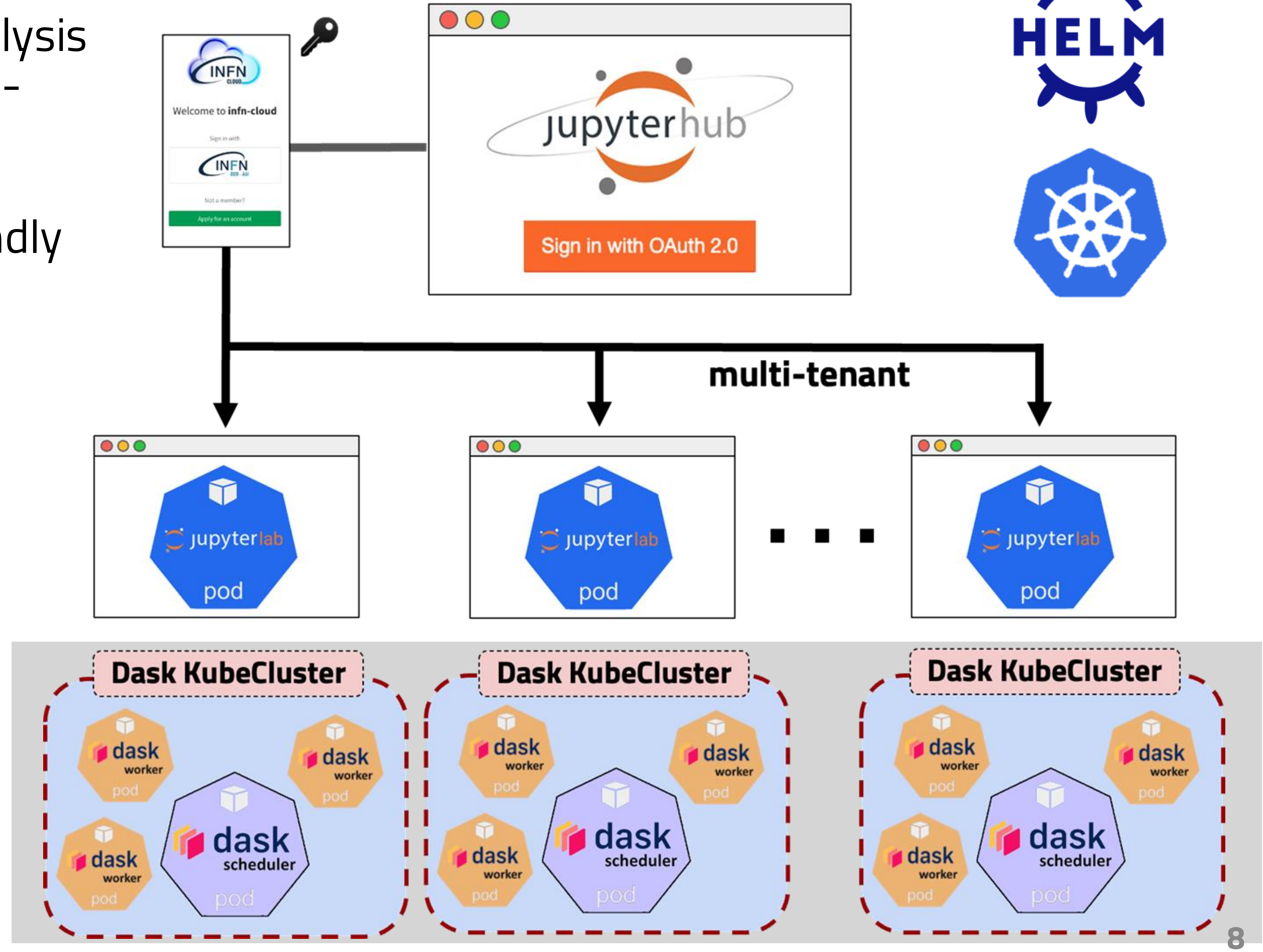
- Ideal environment for testing interactive analysis and validating new frameworks, e.g. the multi-threading features of ROOT RDataFrame

- The Dask Labextension provides a user-friendly monitoring dashboard

- More in the official docs!

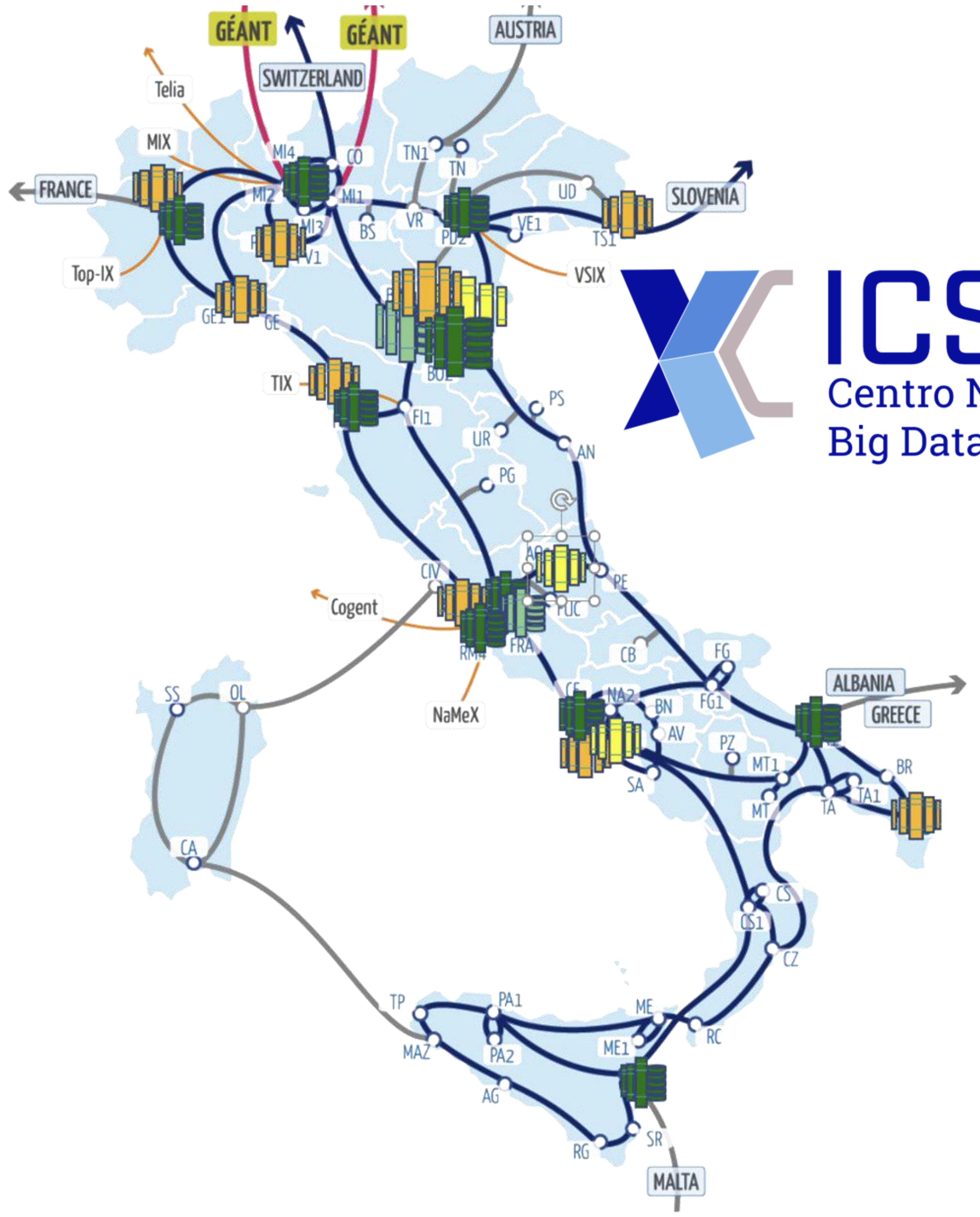
Dask Dashboard 1 **Monitoring workers** 2 **Cluster map**





High throughput data analysis platform

- Offloading strategy: resources used to offload the computation are hosted in the same k8s cluster as the jupyter interface, via DASK KubeCluster
- **Under development:** spawning on multiple remote sites allowing for heterogeneous resources (HTC/HPC/Cloud) (see more in backup)



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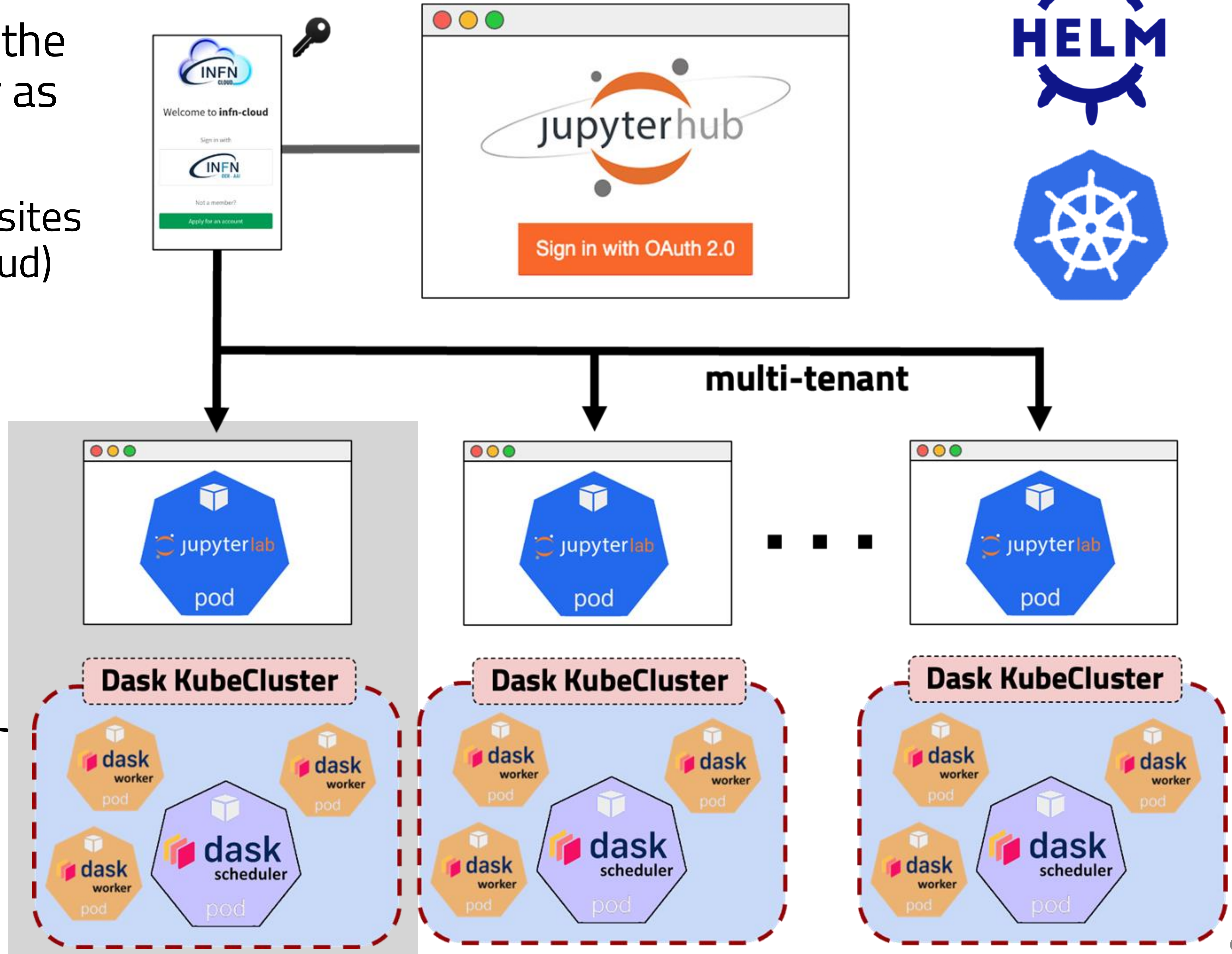
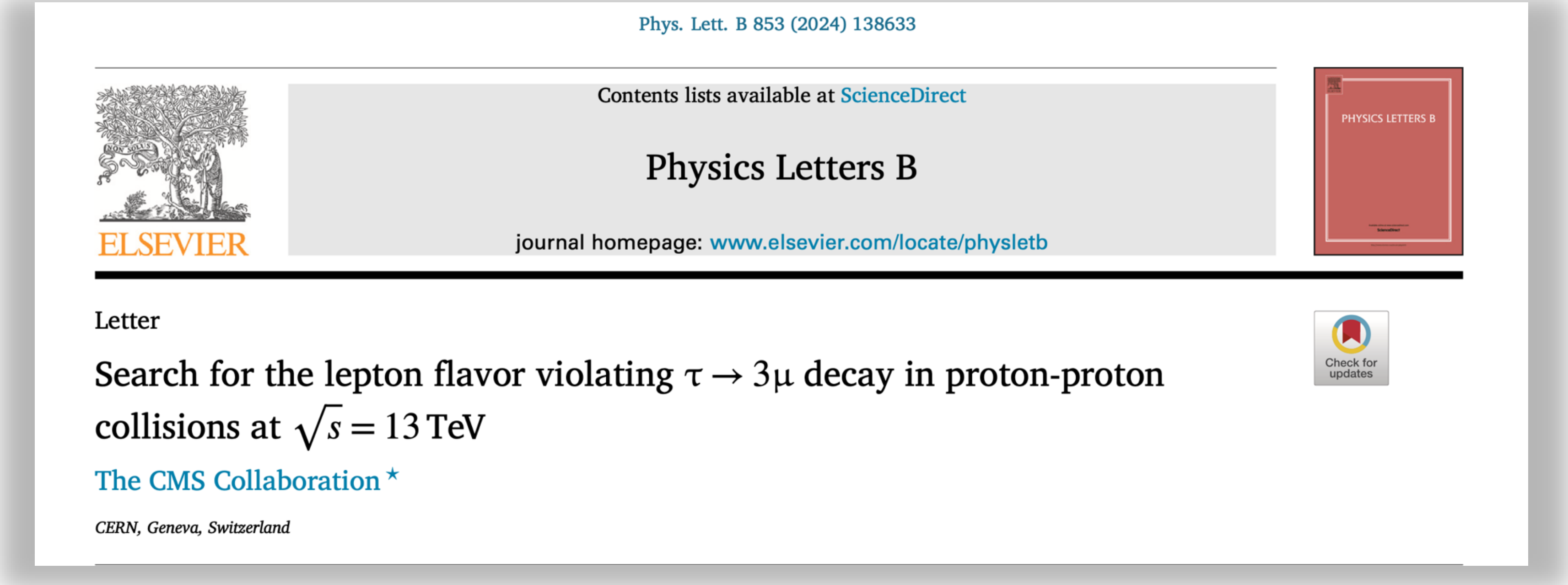
Offloading to..



Benchmark interactive analyses

CMS use-case


Phys. Lett. B 853 (2024) 138633

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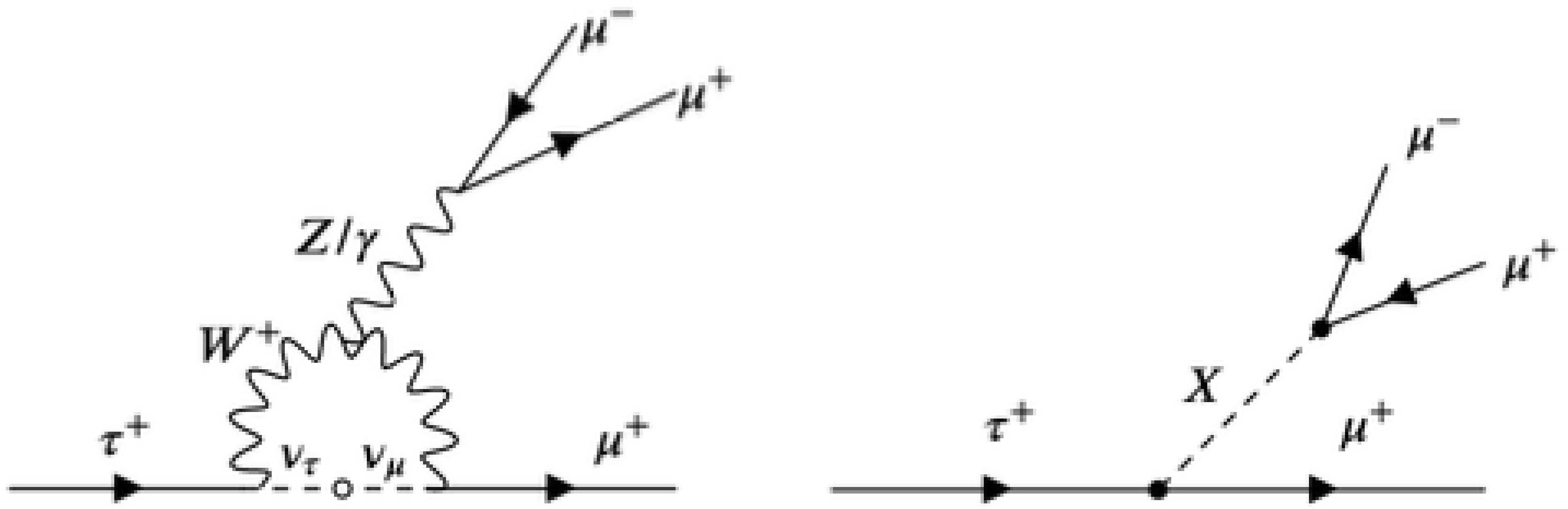
Letter

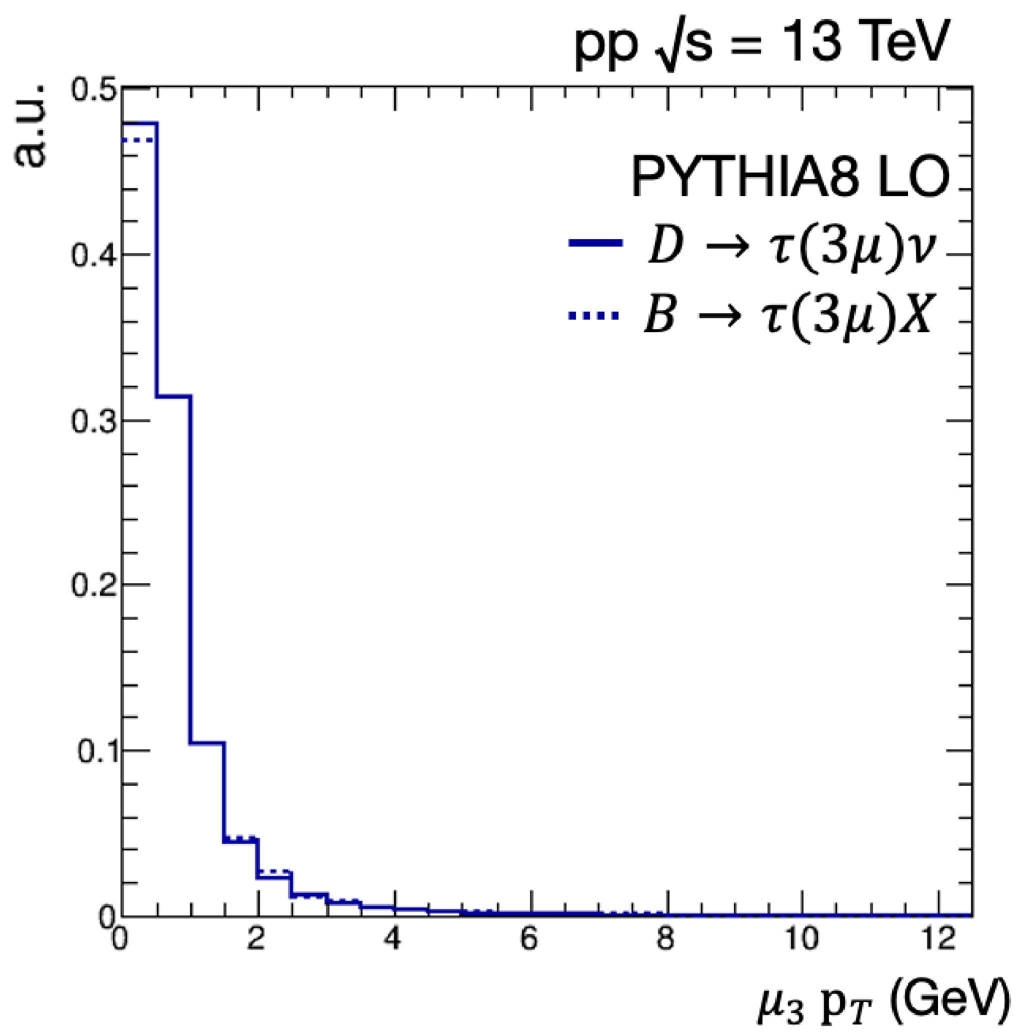
Search for the lepton flavor violating $\tau \to 3\mu$ decay in proton-proton collisions at $\sqrt{s} = 13$ TeV

The CMS Collaboration *

CERN, Geneva, Switzerland

Lepton Flavor Violation in the charged sector: $\tau \to 3\mu$





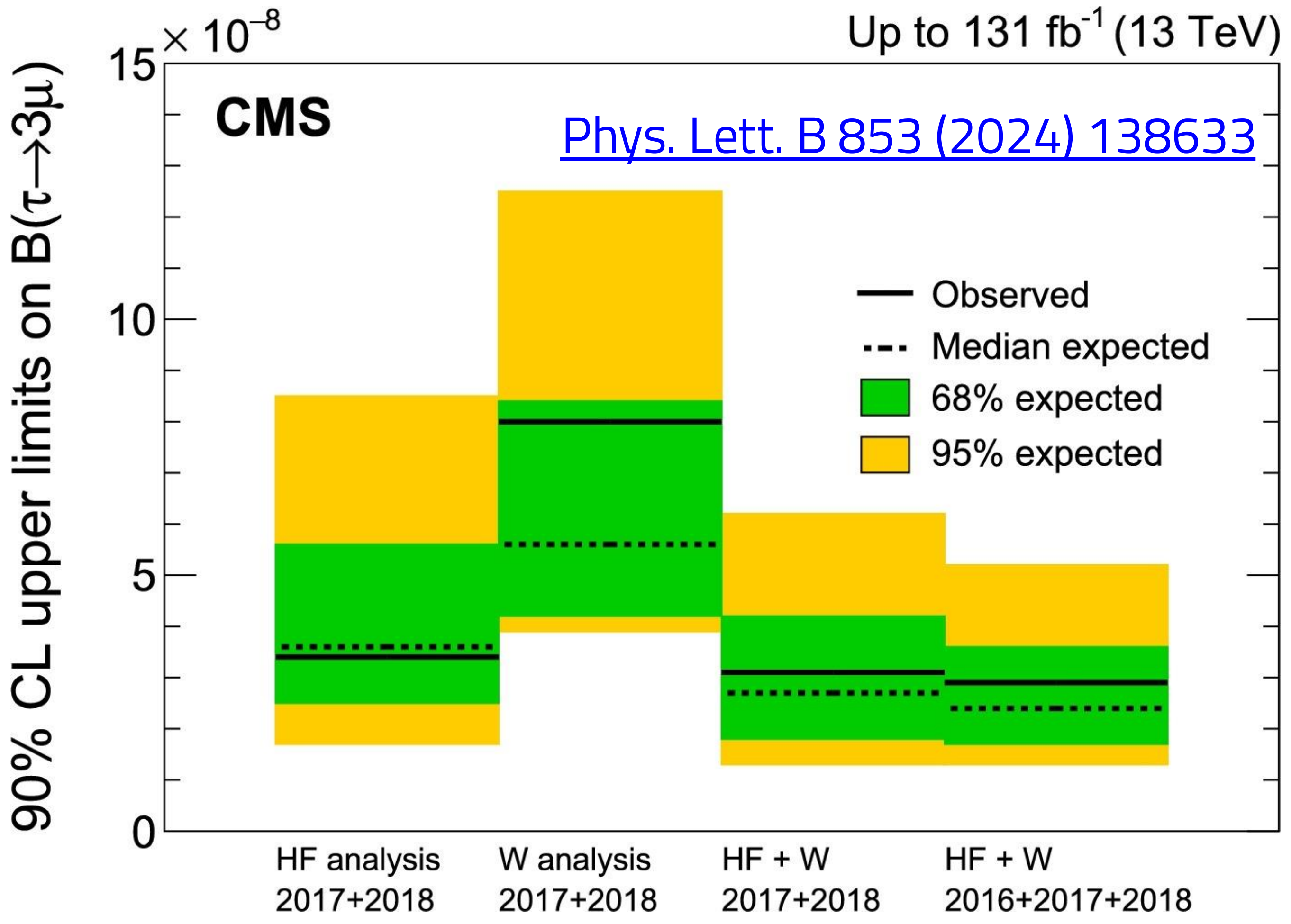
Search for $\boldsymbol{\tau \to 3\mu}$ decays, which have very small SM branching fractions $\mathrm{BR_{SM}} \sim \mathcal{O}(10^{-55})$, while being predicted with sizable BR in several BSM scenarios $\mathrm{BR_{BSM}} \sim \mathcal{O}(10^{-10} \div 10^{-8})$

- $\boldsymbol{\tau}$ leptons produced in D and B meson decays provide large statistics at LHC experiments, but are only accessible with **low-p_T muon triggers**

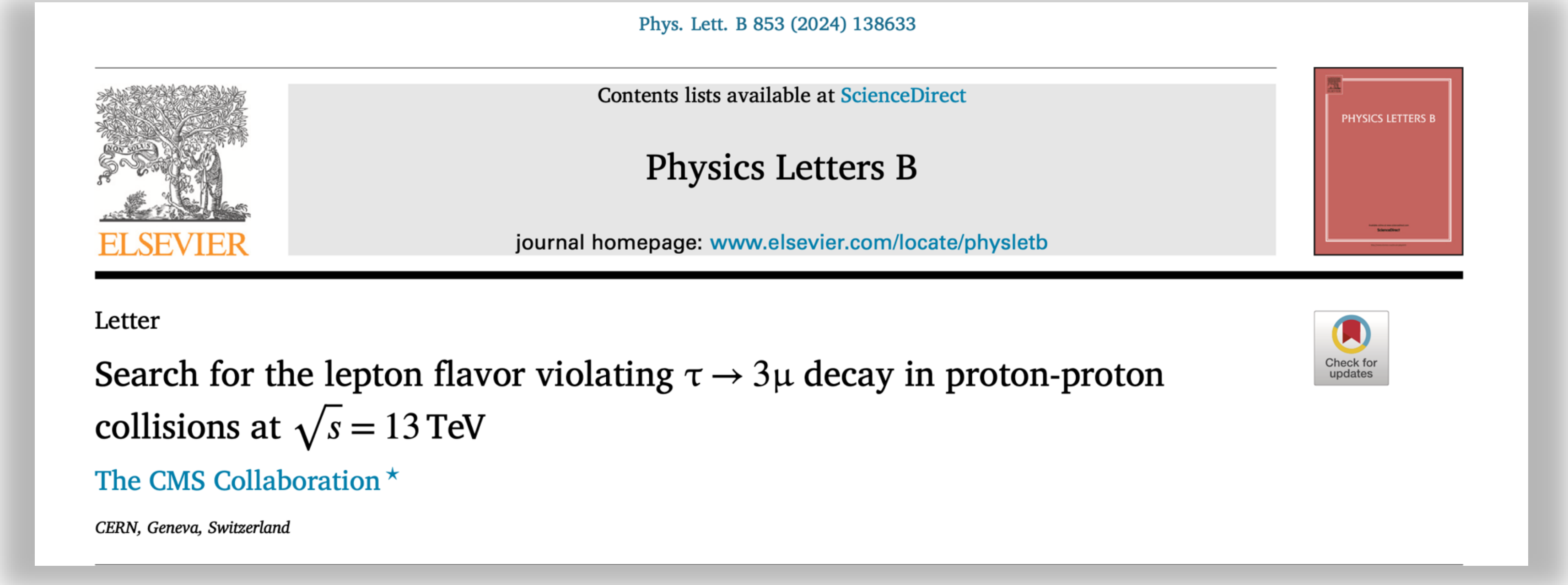
- Analysis of Run 2 data recently published, **stat. limited**

→ benefitting from inclusive low-p_T muon L1 trigger in **Run 3**

→ technical challenge: **new datasets are × 2 ÷ 3 times heavier**



CMS use-case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journal homepage: www.elsevier.com/locate/physletb
Letter
Search for the lepton flavor violating $\tau \to 3\mu$ decay in proton-proton collisions at $\sqrt{s} = 13\,\text{TeV}$
The CMS Collaboration *
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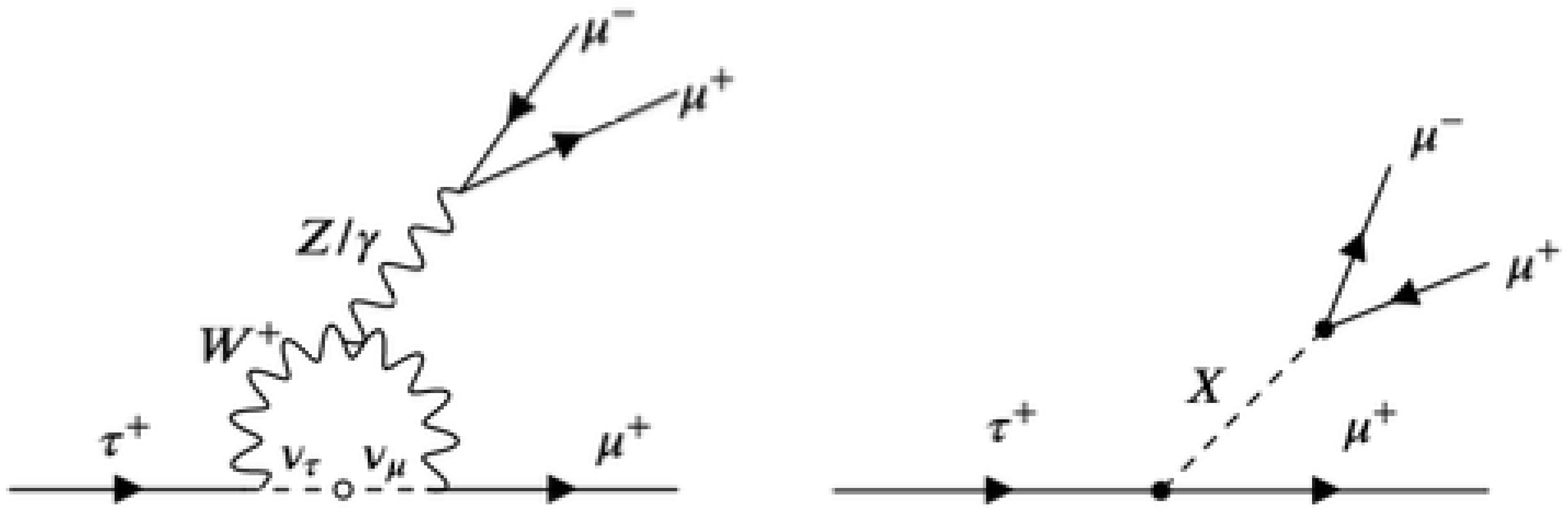
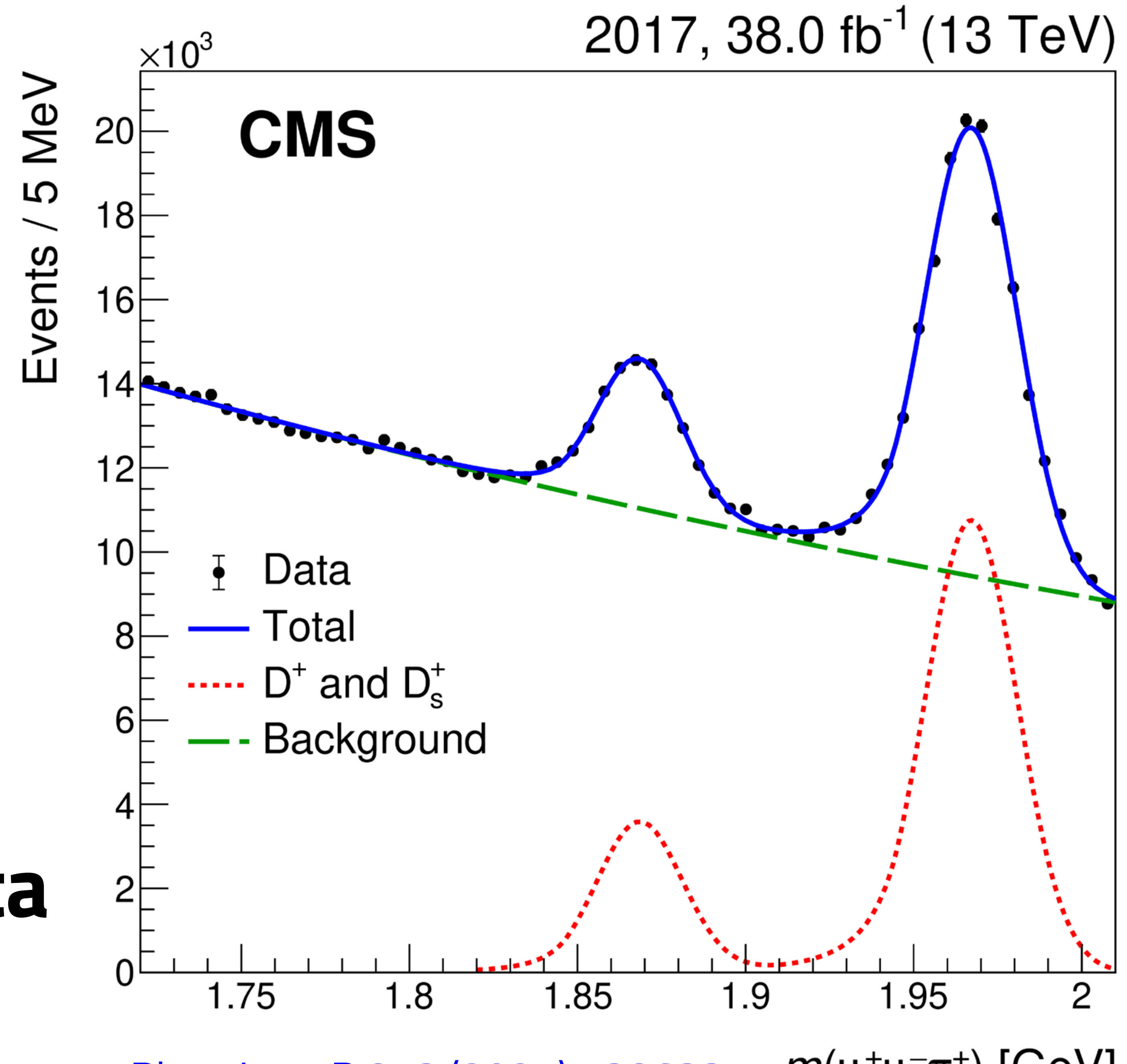
Lepton Flavor Violation in the charged sector: $\tau \to 3\mu$



Search for $\boldsymbol{\tau \to 3\mu}$ decays, which have very small SM branching fractions $\mathrm{BR}_{\mathrm{SM}} \sim \mathcal{O}(10^{-55})$, while being predicted with sizable BR in several BSM scenarios $\mathrm{BR}_{\mathrm{BSM}} \sim \mathcal{O}(10^{-10} \div 10^{-8})$

- $\boldsymbol{\tau}$ leptons produced in D and B meson decays provide large statistics at LHC experiments, but are only accessible with **low-p_T muon triggers**
- The normalisation channel used as a benchmark: $D_s^+ \to \phi(\mu\mu)\pi^+$

→ **cut-based analysis + mass fit for measuring the D_s^+ yield in data**



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$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis workflow

CMS Dataset

- Data collected by low p_T dimuon triggers
- MiniAOD data tier **centrally produced**

ROOT ntuples

- **Skimmed** data, events with 2μ+1track final state
- Saving only physics objects of interest
- **Plain data format**, ~ 5 GB / fb-1, stored on eos

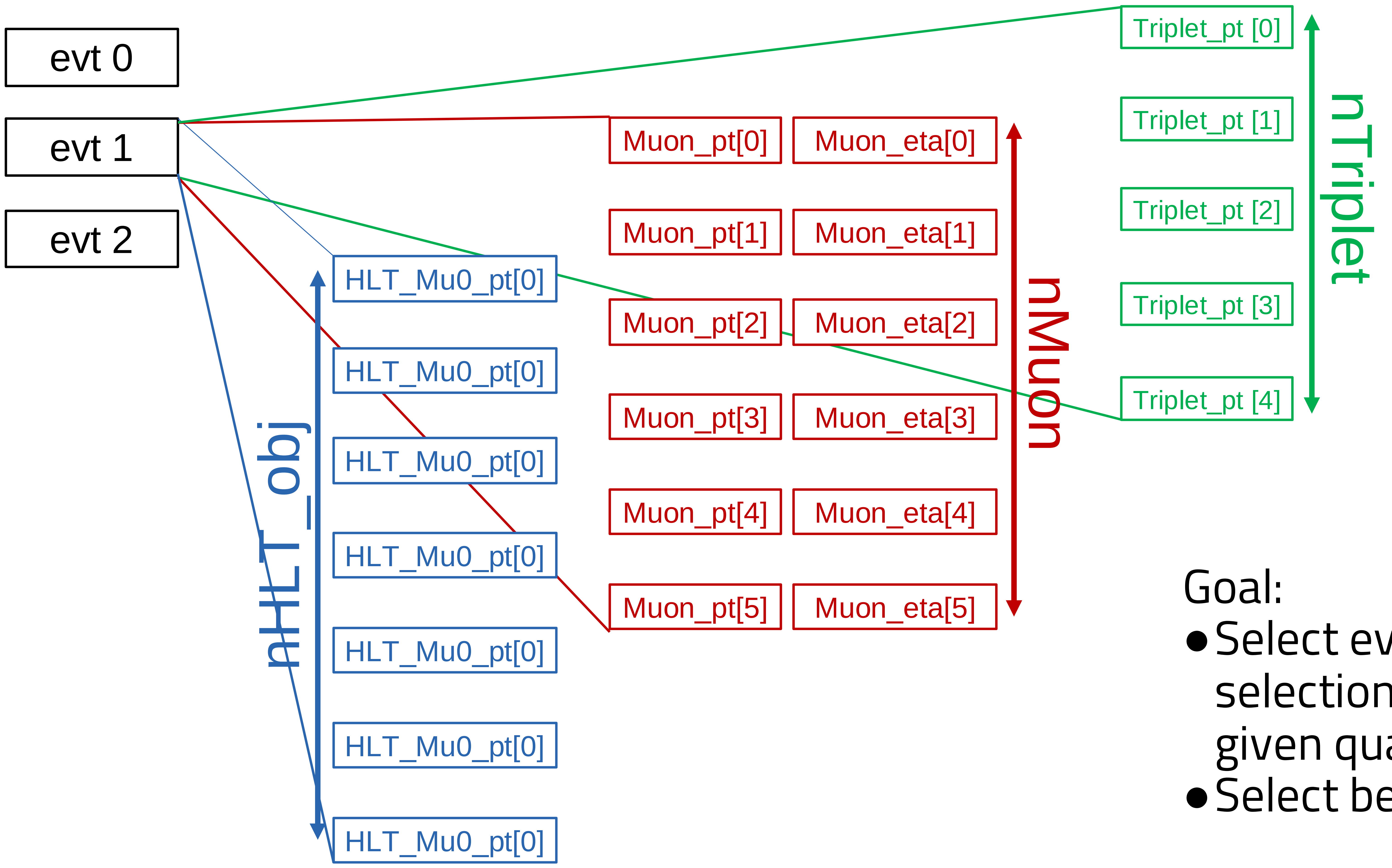
Analysis

- Define **high-level variables**
- Apply **scale factors** and corrections
- Apply **selections**, select best D_s candidate per event
- **Fit** the 2μ+1track invariant mass

- **Legacy: approach** Loop-based analysis implemented using ROOT TTree:MakeClass
  - split computation in batches of input files, run separately as HTCondor jobs, gather the output rootfiles

- **New**: Ntuples read as RDataFrame, almost all operations “lazy” → no loop triggered till the end
  - going distributed using ROOT RDataFrame distributed features, with Dask backend.

Ntuples are nanoAOD-like



Goal:
- Select events with triplets passing selections (e.g. containing muons with a given quality)
- Select best triplet per event in case >1 pass

$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis code

Basic imports

[1]:
```python
import sys, os, time
start = time.time()
import json
import ROOT
```

```
Welcome to JupyROOT 6.30/02
```

Dask scheduler

[2]:
```python
from dask.distributed import Client, performance_report
```

[3]:
```python
Local = False

if Local:
    from dask.distributed import LocalCluster
    cluster = LocalCluster()
    client = Client(cluster.scheduler.address)
```

Now start new Dask cluster, scale the number of workers

[5]:
```python
# fill this cell with "<>" button of Dask labextension
```

[4]:
```python
from dask.distributed import Client

client = Client("tcp://dask-simonef-80b8d6c6-2-scheduler.jhub:8786")
client
```

[4]:

Client

Client-32e794b5-908b-11ef-82a4-3ee1209b75b0

Connection method: Direct

Dashboard: http://dask-simonef-80b8d6c6-2-scheduler.jhub:8787/status

Launch dashboard in JupyterLab

▸ Scheduler Info

- Define a Dask Client

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$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis code

- Define a Dask Client
- Load X509 user proxy to Dask workers and set env paths

X509 proxy configuration

The `/tmp/x509up_u` file should be generated prior running the notebook using `voms-proxy-init -cert ../cert/usercert.pem -key ../cert/userkey.pem`

```
[9]: from distributed.diagnostics.plugin import UploadFile
     client.register_worker_plugin(UploadFile("/tmp/x509up_u0"))
```

```
/tmp/ipykernel_676/2847743139.py:2: DeprecationWarning: `Client.register_worker_plugin` has
been deprecated; please use `Client.register_plugin` instead
  client.register_worker_plugin(UploadFile("/tmp/x509up_u0"))
```

```
[9]: {'tcp://10.42.0.75:43259': {'status': 'OK'},
      'tcp://10.42.0.76:42581': {'status': 'OK'},
      'tcp://10.42.1.93:32875': {'status': 'OK'},
      'tcp://10.42.1.94:42729': {'status': 'OK'},
      'tcp://10.42.2.68:41105': {'status': 'OK'},
      'tcp://10.42.2.69:41157': {'status': 'OK'},
      'tcp://10.42.3.92:36155': {'status': 'OK'},
      'tcp://10.42.3.93:34933': {'status': 'OK'},
      'tcp://10.42.3.94:43541': {'status': 'OK'},
      'tcp://10.42.4.76:42331': {'status': 'OK'},
      'tcp://10.42.4.77:38303': {'status': 'OK'},
      'tcp://10.42.4.78:43961': {'status': 'OK'},
      'tcp://10.42.4.79:45559': {'status': 'OK'},
      'tcp://10.42.6.89:34275': {'status': 'OK'},
```

```
[10]: def set_proxy(dask_worker):
          import os
          import shutil
          working_dir = dask_worker.local_directory
          proxy_name = 'x509up_u0'
          os.environ['X509_USER_PROXY'] = working_dir + '/' + proxy_name
          os.environ['X509_CERT_DIR']="/cvmfs/grid.cern.ch/etc/grid-security/certificates/"
          return os.environ.get("X509_USER_PROXY"), os.environ.get("X509_CERT_DIR")
```

```
[11]: client.run(set_proxy)
```

```
[11]: {'tcp://10.42.0.75:43259': ('/tmp/dask-scratch-space/worker-ee12y_1w/x509up_u0',
        '/cvmfs/grid.cern.ch/etc/grid-security/certificates/'),
       'tcp://10.42.0.76:42581': ('/tmp/dask-scratch-space/worker-lp8yzbsh/x509up_u0',
        '/cvmfs/grid.cern.ch/etc/grid-security/certificates/'),
```

$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis code

Declare custom C++ functions

```
[8]: text_file = open("Utilities.h", "r")
data = text_file.read()


def my_initialization_function():
    ROOT.gInterpreter.Declare('{}'.format(data))

ROOT.RDF.Experimental.Distributed.initialize(my_initialization_function)
```

```
numWorkers= len(client.scheduler_info()['workers'])
#npartitions = 2 * numWorkers
npartitions = 2 * nfiles

print("Number of workers is: {}".format(numWorkers))
print("Number of total partitions is: {}".format(npartitions))

df = ROOT.RDF.Experimental.Distributed.Dask.RDataFrame(treename, chain, daskclient=client)
```

'root://eosuser.cern.ch//eos/mypath/*.root'

- Define a Dask Client
- Load X509 user proxy to Dask workers and set env paths
- Declare useful C++ functions and define Distributed.Dask.RDataFrame

$D_s^+ \rightarrow \phi(\mu\mu)\pi^+$ analysis code

```
# Selections on triplets
# 2 -> 2mu+track candidate mass in (1.62-2.02)GeV
# 3 -> at least 2 track associated with PV
# 4 -> Significance of BS-SV distance in the transverse plane > 2
triplet_selection = "Triplet2_Mass>1.62 && Triplet2_Mass<2.02 && \
                     RefittedPV2_NTracks > 1 && \
                     FlightDistBS_SV_Significance > 2 "

# Events with at least one good candidate
df = df.Define("triplet_mask1", triplet_selection).Filter("ROOT::VecOps::Sum(triplet_mask1) >0")
```

- Define a Dask Client
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- Declare useful C++ functions and define Distributed.Dask.RDataFrame

Some steps of the analysis:

- Apply selections on branches with size nTriplet

$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis code

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- Match other branches (e.g. Muon_*) with Triplet_* and apply selections

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# Events with at least one good candidate
df = df.Define("triplet_mask1", triplet_selection).Filter("ROOT::VecOps::Sum(triplet_mask1) >0")
```

```
# Find index in "Muon_" and "Track_" branches
df = df.Define("Mu01_index", "match(MuonPt, Mu01_Pt)")
df = df.Define("Mu02_index", "match(MuonPt, Mu02_Pt)")
df = df.Define("Tr_index",   "match(MuonPt, Tr_Pt)")

# 7 -> Apply Muon ID Global and Particle Flow
df = df.Define("Mu01_ID", "muon_id(Mu01_index, Muon_isGlobal && Muon_isPF)")
df = df.Define("Mu02_ID", "muon_id(Mu02_index, Muon_isGlobal && Muon_isPF)")

# 8 -> IP(track, BS) z direction < 20 cm and xy direction < 0.3 cm
df = df.Define("Tr_IPcut", "muon_id(Tr_index, (Track_dz<20 && Track_dxy<0.3) )")
df = df.Define("triplet_mask4", "Mu01_ID && Mu02_ID && Tr_IPcut").Filter("ROOT::VecOps::Sum(triplet_mask4)>0")
```

```
RVec<int> match(ROOT::VecOps::RVec<double> branch1, ROOT::VecOps::RVec<double> branch2){
//returns vector of indeces such that branch2[index]=branch1
    RVec<int> index;
    for(unsigned i = 0; i<branch1.size(); i++){
      auto idx = std::find(branch2.begin(), branch2.end(), branch1.at(i));
      if( idx != branch2.end()) index.push_back(std::distance(branch2.begin(), idx));
      else index.push_back(-99);
    }
    return index;
}
```

$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis code

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```

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df = df.Define("triplet_mask4", "Mu01_ID && Mu02_ID && Tr_IPcut").Filter("ROOT::VecOps::Sum(triplet_mask4)>0")
```

- Define a Dask Client
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- Declare useful C++ functions and define Distributed.Dask.RDataFrame

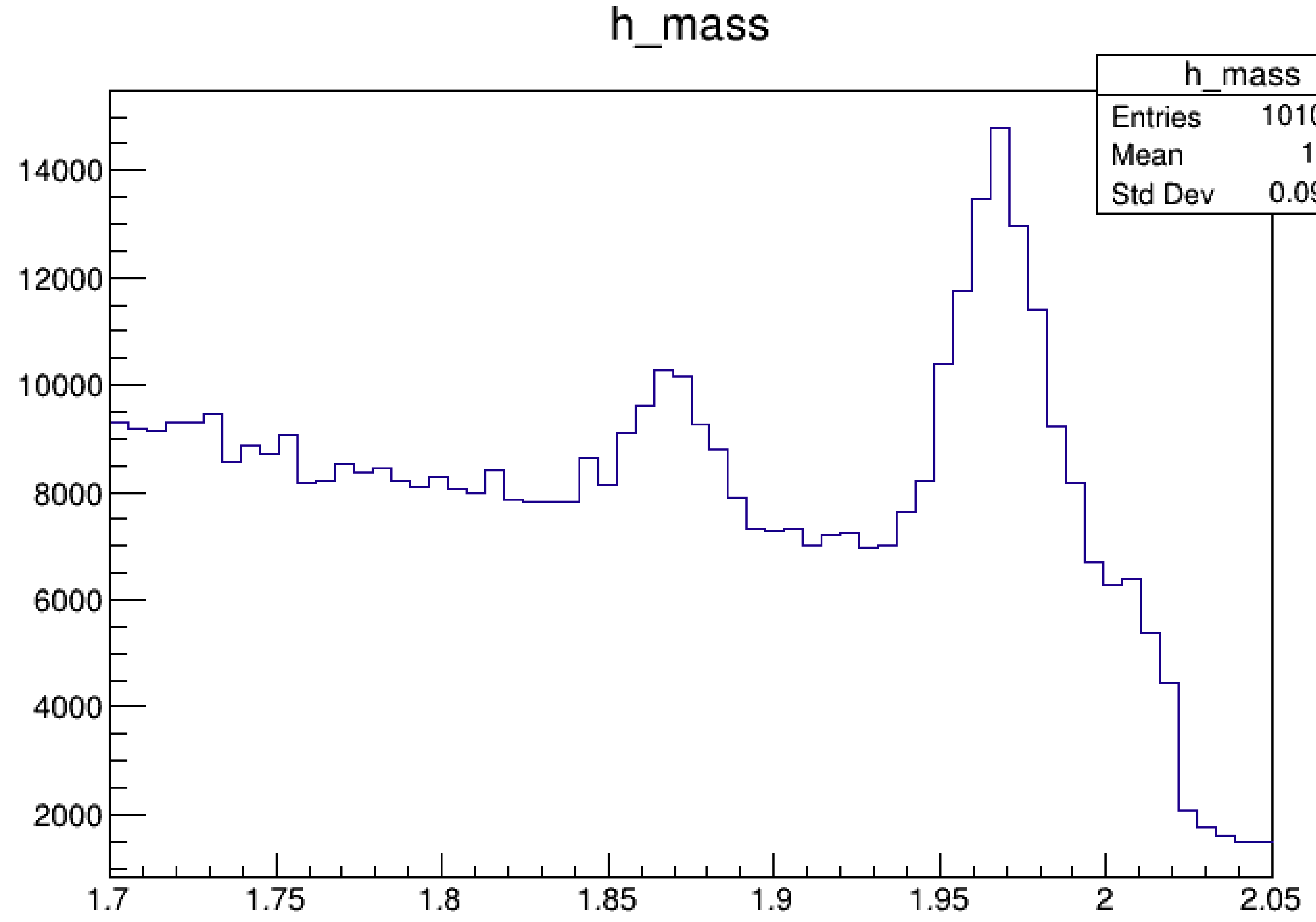
Some steps of the analysis:

- Apply selections on branches with size nTriplet
- Match other branches (e.g. Muon_*) with Triplet_* and apply selections
- Keep best mu mu track candidate

```
# Keep best candidate based on vertex chi2
df = df.Define("BestTriplet_index", "bestcandidate(TripletVtx2_Chi2)")
df = df.Define("BestTriplet_mass", "flattening(Triplet2_Mass, BestTriplet_index)")
```

$D_s^+ \to \phi(\mu\mu)\pi^+$ analysis code

```
# Create a histogram from `x` and draw it
with performance_report(filename="my_report.html"):
  h = df.Histo1D(("h_mass", "h_mass", 62, 1.70, 2.05), "BestTriplet_mass")
  c =  ROOT.TCanvas()
  h.Draw("hist")
  c.Draw()
```




```
# Save output for further processing: snapshot saves on workers!
df_out = df.Snapshot("ntuple", "out.root", ["BestTriplet_mass"])

np_out = df.AsNumpy(columns=["BestTriplet_mass"]) #workers stay "in-memory" forever
```

- Define a Dask Client
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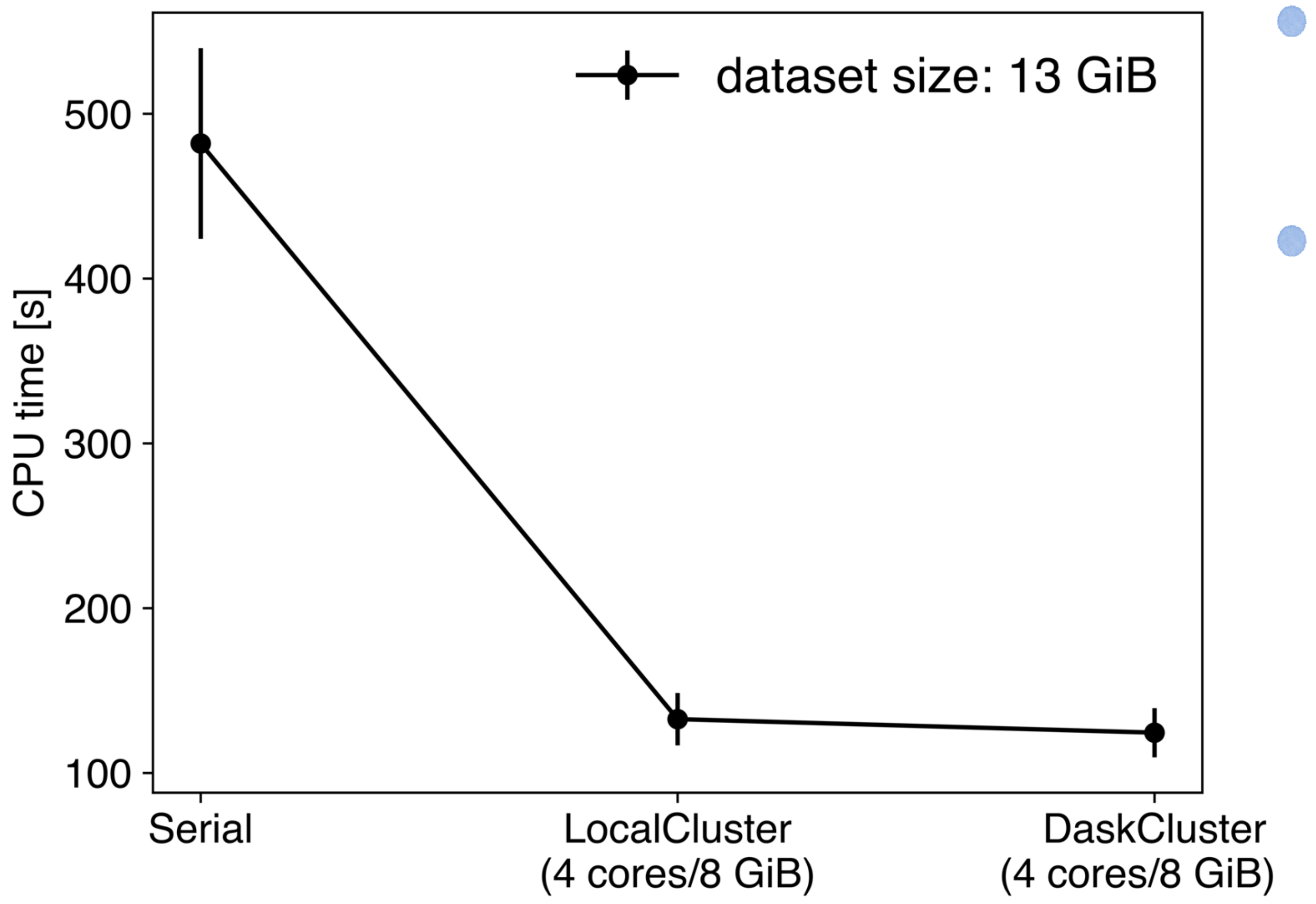
Some steps of the analysis:
- Apply selections on branches with size nTriplet
- Match other branches (e.g. Muon_*) with Triplet_* and apply selections
- Keep best mu mu track candidate

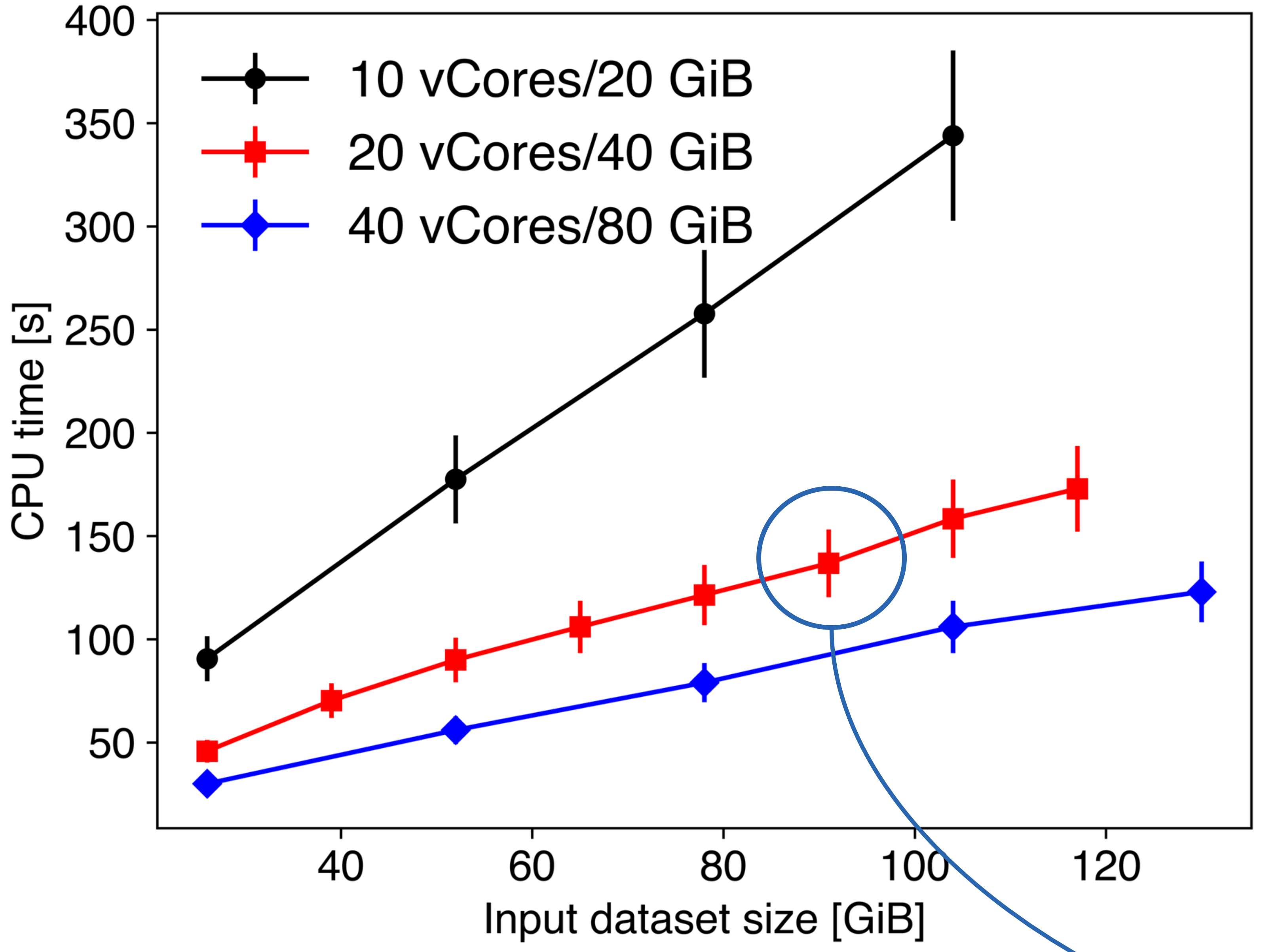
Output/results:
- Drawing or counting out of the final df triggers the computation → smooth
- Snapshoting the final df for further analysis: many "out.root" files are saved in the workers and need to be copied back
- Tried "AsNumpy" as an alternative → workers don't finish computation

Preliminary results



- Significant improvement in execution time *wrt* the standard/serial approach
- The facility allows for dynamically scaling the resources, here testing the performance at fixed #cores and memory, varying the dataset size

- Stress test at high CPU and memory occupancy
- Stable performance, linearly scaling with the input dataset size
- Dataset size ~ 100 GiB is representative of ~15 /fb of Run3 data for this specific analysis



Feedback from a user point of view:

- Implementing the analysis in RDataFrame was easy, looking at tutorials and forum
- Interfacing RDataFrame and Dask → only few lines of code, no debugging needed
- It would be nice to have a “distributed” version of Snapshot for harvesting the outputs from the workers (or maybe I missed something here? ☺)

- This AF is under testing, we presently have ~10 beta users from CMS, ATLAS, FCC (mostly from CMS tough)
- Will reach a larger audience after expanding the current pool of resources

Conclusions & Next Steps

- HL-LHC poses significant challenges to HEP experiments in terms of storage and computing resources
- An interactive high throughput platform has been developed in the framework of the "HPC, Big Data e Quantum Computing Research Centre" Italian National Center (ICSC)
  - offers users a modern interactive web interface based on JupyterLab
  - experiment-agnostic resources
  - based on a parallel and geographically distributed back-end

- Interactive analyses feasibility studies on INFN cloud succeeded
  - Performance evaluated using the high-rate platform
  - HEP analysis use-case explored from the CMS and ATLAS Collaborations

Medium-long term goals: Expand the current pool of resources by a factor of 5 in the upcoming months, to perform scale testing of the analysis workflows.

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Thank you!

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Back-up

High throughput data analysis platform

- Offloading strategy: resources used to offload the computation are hosted in the same k8s cluster as the jupyter interface, via DASK KubeCluster

- **Under development:** schedule worker processes spawning on multiple remote sites dynamically and transparently → Implementation on heterogeneous resources (HTC/HPC/Cloud)

InterLink provides execution of a Kubernetes pod on almost any remote resource. Resources visible to the user thanks to an HTCondor overlay