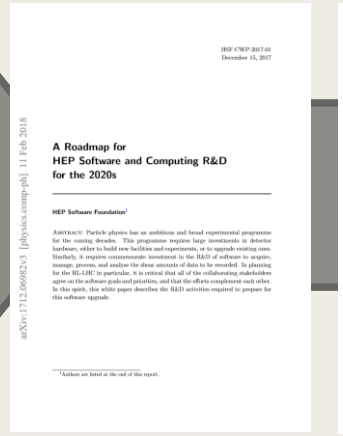
IRIS-HEP

G. Watts (UW/Seattle)
For the IRIS-HEP Team

Community White Paper



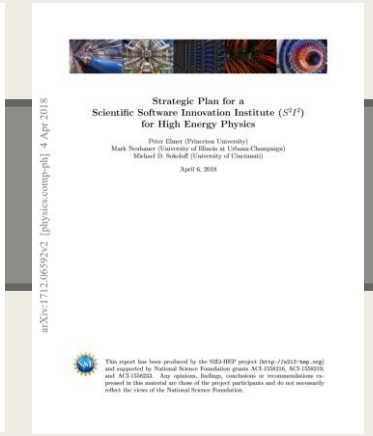
HSF-CWP-2017-01
December 15, 2017

A Roadmap for
HEP Software and Computing R&D
for the 2020s

HEP Software Foundation[1]

Abstract: Particle physics has an ambitious and broad experimental programme for the coming decades. This programme requires large investments in detector hardware, either to build new facilities and experiments, or to upgrade existing ones. Similarly, it requires commensurate investment in the R&D of software to acquire, manage, process, and analyse the shear amounts of data to be recorded. In planning for the HL-LHC in particular, it is critical that all of the collaborating stakeholders agree on the software goals and priorities, and that the efforts complement each other. In this spirit, this white paper describes the R&D activities required to prepare for this software upgrade.

[1]Authors are listed at the end of this report.



Strategic Plan for a
Scientific Software Innovation Institute (S^2I^2)
for High Energy Physics

Peter Elmer (Princeton University)
Mark Neubauer (University of Illinois at Urbana-Champaign)
Michael D. Sokoloff (University of Cincinnati)

April 6, 2018

This report has been produced by the S2I2-HEP project (http://s2i2-hep.org) and supported by National Science Foundation grants ACI-1558516, ACI-1558519, and ACI-1558233. Any opinions, findings, conclusions or recommendations expressed in this material are those of the project participants and do not necessarily reflect the views of the National Science Foundation.

iris hep
Institute for Research & Innovation
in Software for High Energy Physics

Community White Paper

2016-2017

Involved A Diverse Group

- Computing Management from the Experiments and Labs
- Individuals interested in the problems
- Members of other compute intensive scientific endeavors
- Members of Industry

Individual Papers on the arXiv:

Careers & Training, Conditions Data, DOMA, Data Analysis & Interpretation, Data and Software Preservation, Detector Simulation, Event/Data Processing Frameworks, Facilities and Distributed Computing, Machine Learning, Physics Generators, Security, Software Development, Deployment, Validation, Software Trigger and Event Reconstruction, Visualization

Community White Paper & the Strategic Plan

CWP Topics touched by IRIS-HEP

- Physics Generators
- Machine Learning
- Visualization
- Detector Simulation
- DOMA
- Software Development, Deployment, Validation, Verification
- Software Trigger & Event Reconstruction
- Data-Flow Processing Framework
- Data and Software Preservation
- Data Analysis & Interpretation
- Conditions Data
- Security
- Training

CWP Topics touched by IRIS-HEP

Physics Generators

Machine Learning

Visualization

Detector Simulation

DOMA

Software Development, Deployment, Validation, Verification

Software Trigger & Event Reconstruction

Data-Flow Processing Framework

Data and Software Preservation

Data Analysis & Interpretation

Conditions Data

Security

Training

Areas of large investment

Effort Overview

Area	FTE
Mgmt/Project office	1.6
Analysis Systems	5.2
DOMA	3.6
Innovative Algorithms	9.8
Sustainability Core	0.7
SSL	1.5
OSG-LHC	5.5
Total	**27.9**

A mix of career stages and job categories:

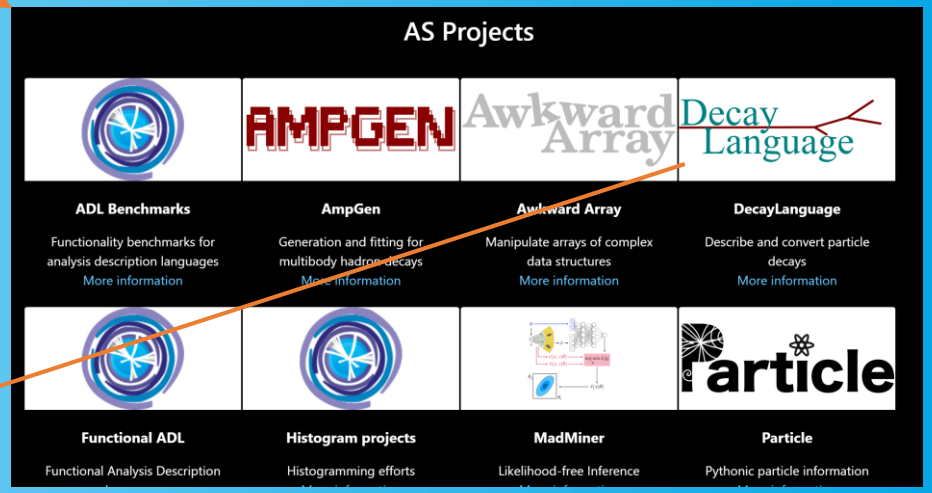
- 12 students ~ 4.6 FTE
- 8.4 FTE postdocs
- 13.7 FTE staff/professionals
- 1.2 FTE faculty

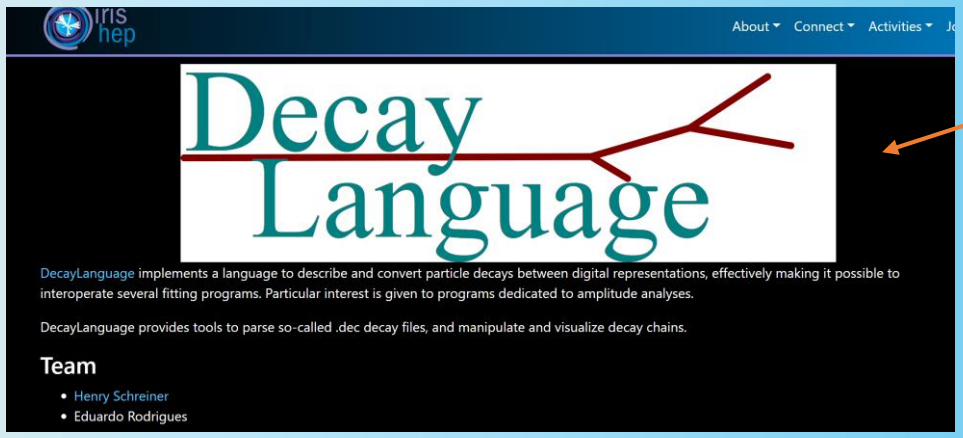
The $5M/year budget goes almost entirely towards salaries (+ travel/M&S/tuition). There is only a very, very modest hardware budget. We aim to leverage that from other sources. There are participant funds (~$80k/year) to support aspects of the intellectual hub activities, blueprint, training, etc.

Where to look for more details

http://iris-hep.org

Almost all projects are detailed on our website



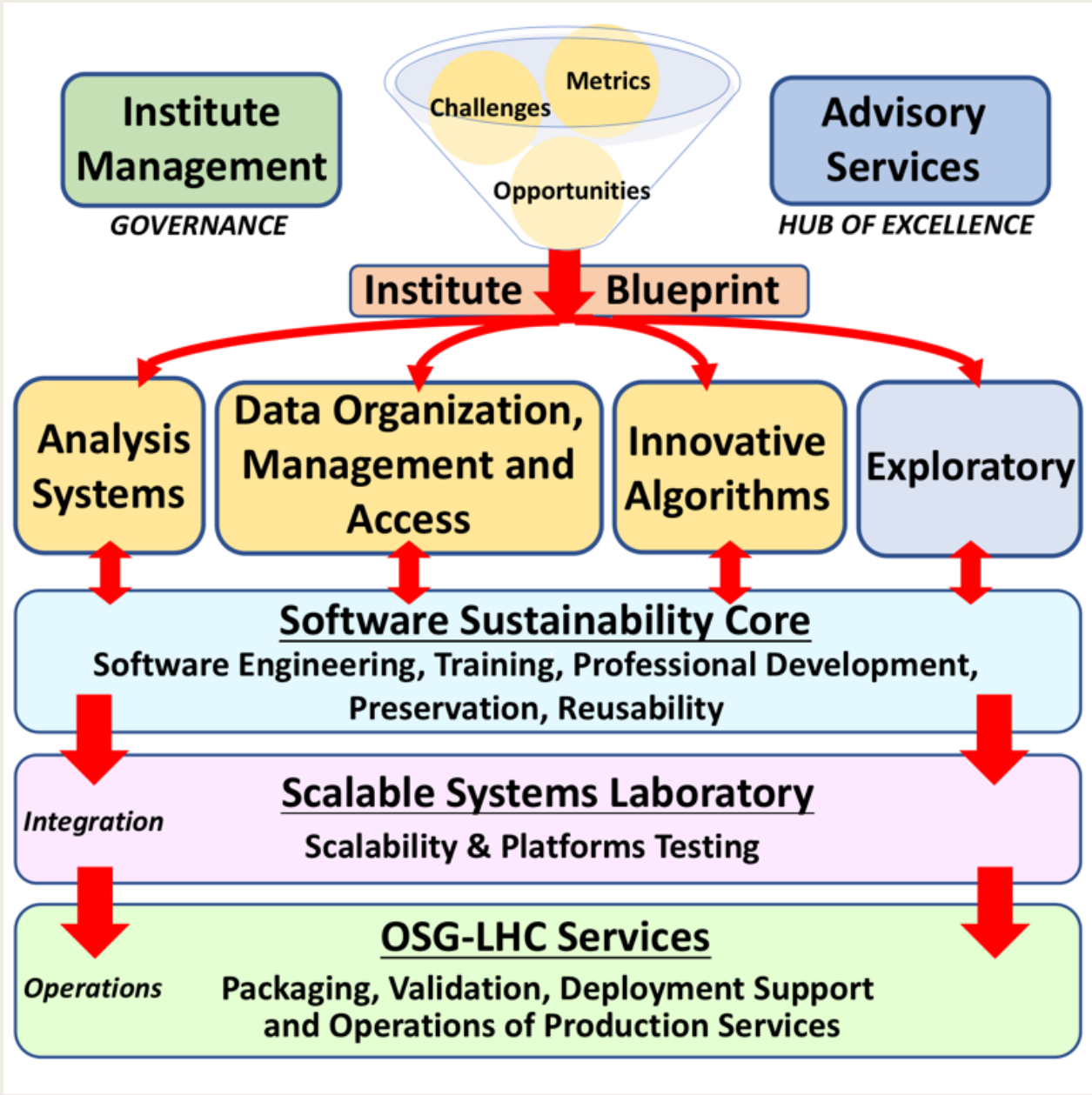


Organization

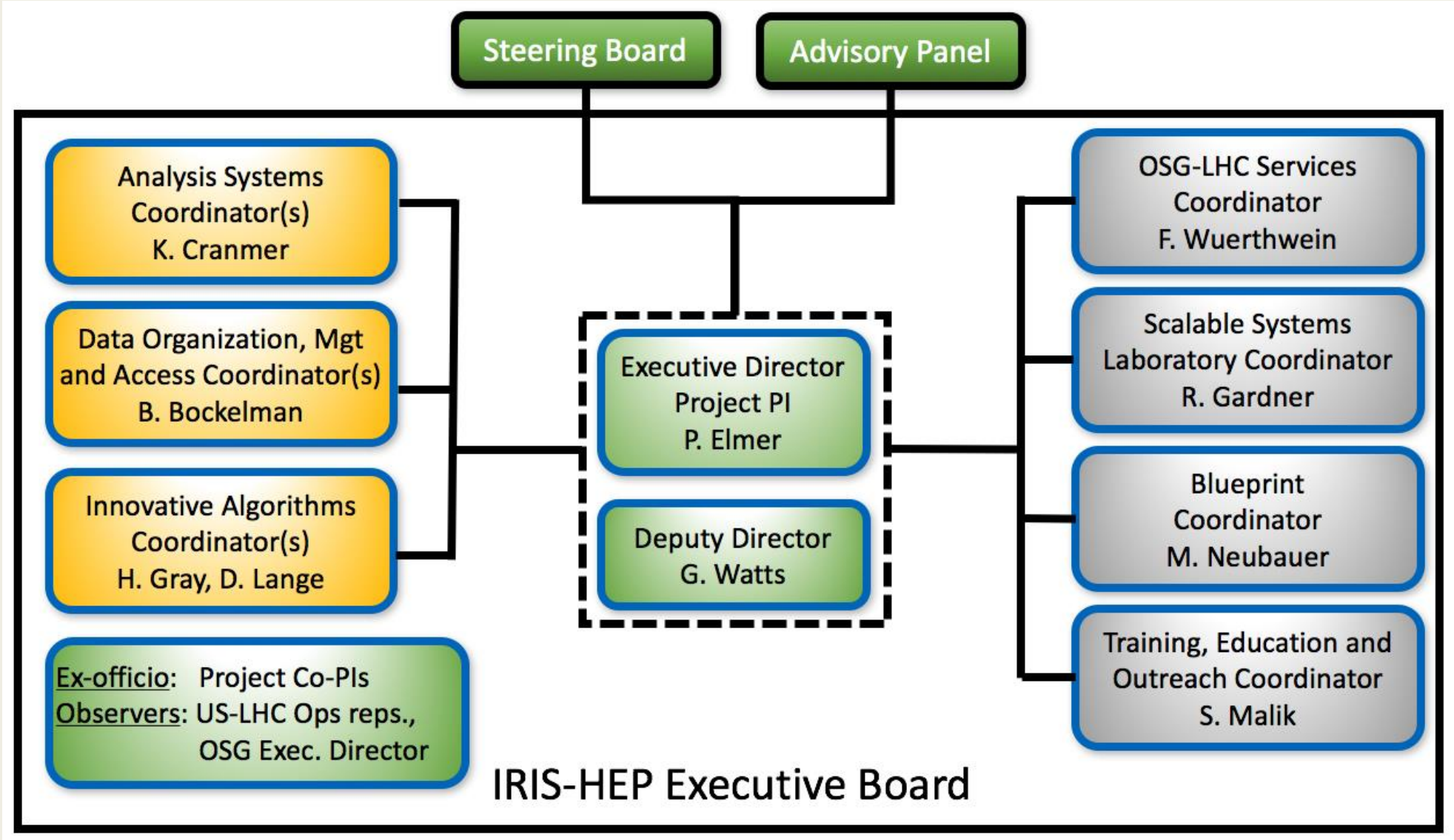
Primary R&D

R&D and Community Support

Production



Management and Coordination



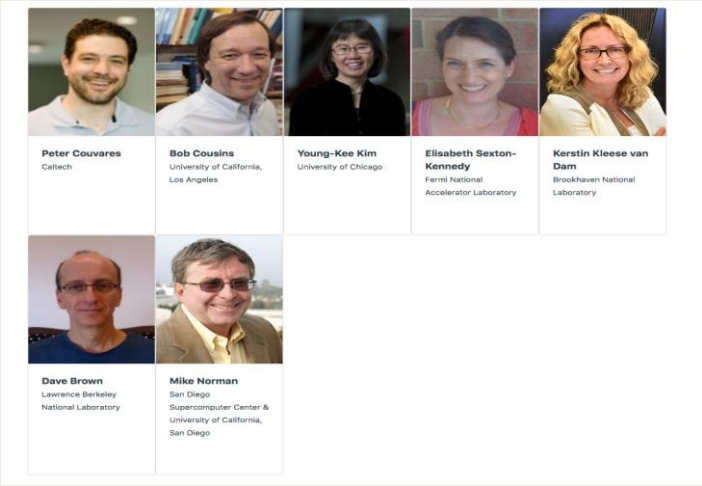
Steering Board and Advisory Panel

Steering Board

Represents the major stakeholders and partners for the IRIS-HEP project. Will meet quarterly with the IRIS-HEP Executive Board to learn the status of the project and **provide feedback on the large scale priorities** and current strategy of the Institute. Members will include representatives from (1) the ATLAS experiment, (2) the CMS experiment, (3) the LHCb experiment, (4) the US-ATLAS Operations program, (5) the US-CMS Operations program, (6) the OSG Council, (7) the Worldwide LHC Computing Grid (WLCG), and (8) the HEP Software Foundation.

Advisory Panel

Provides annual non-stakeholder feedback on the goals and evolving project plans, and evaluates how well the institute is achieving its overall mission as defined with NSF. The Advisory Panel consists of 7 fixed members with an option of inviting ad-hoc additional members as needed for particular topics.



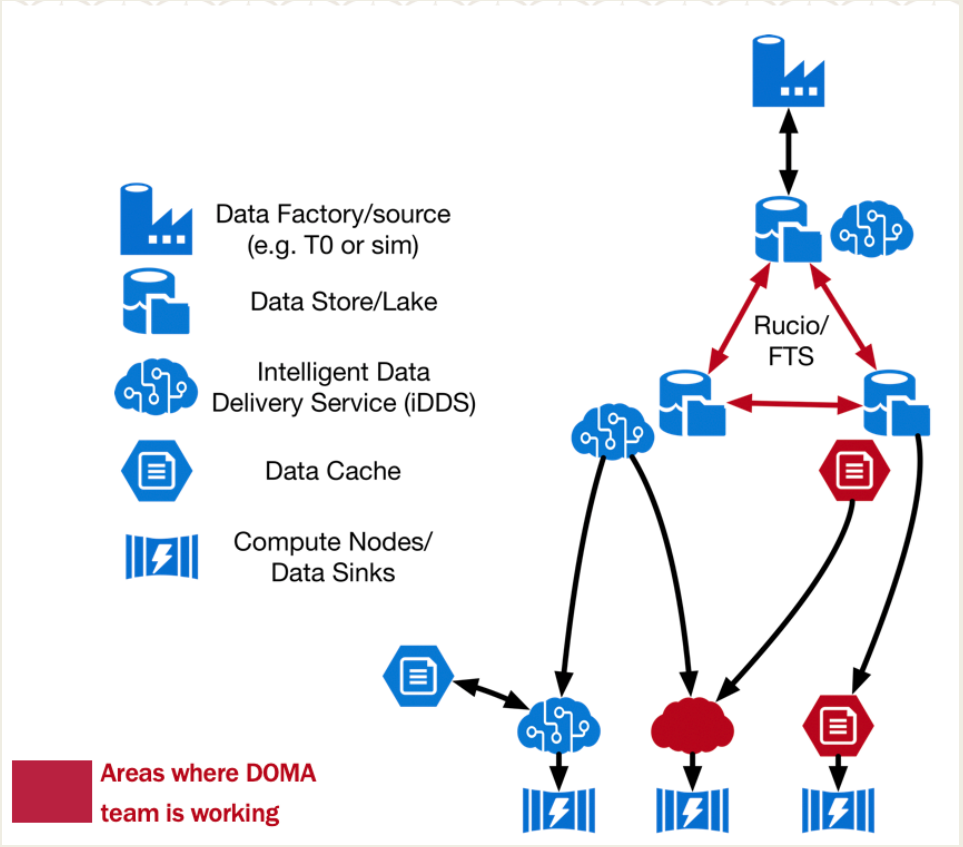
What follows are some highlights

(due to time constraints I will skip most highlights)

Data Organization, Management and Access (DOMA)

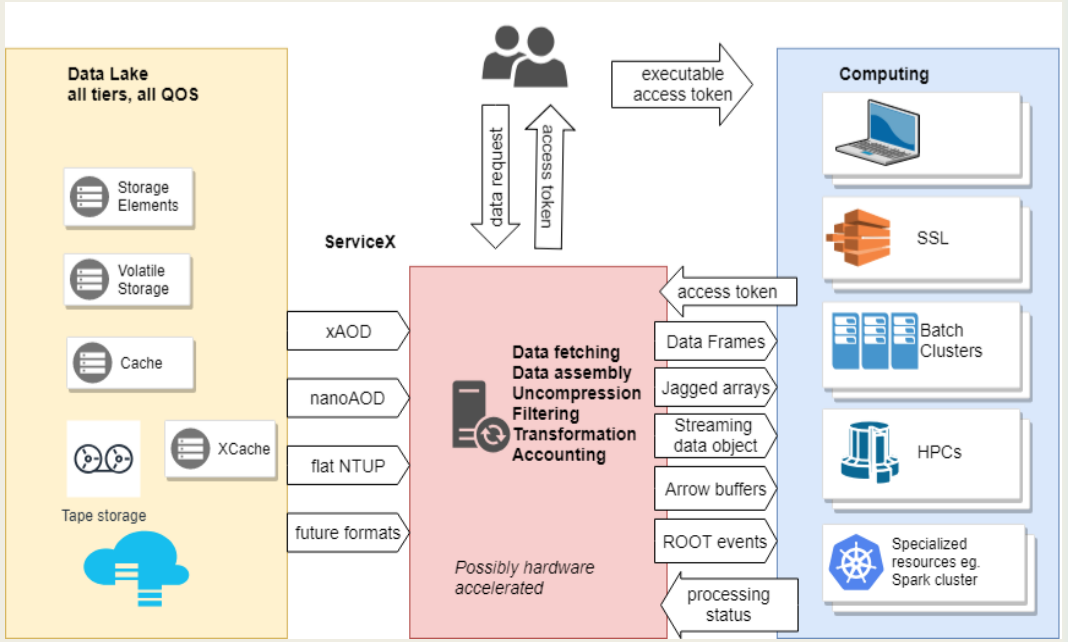
The DOMA focus area performs fundamental R&D related to the central challenges of organizing, managing, and providing access to exabytes of data from processing systems of various kinds.

- **Data Organization**: Improve how HEP data is serialized and stored.
- **Data Access**: Develop capabilities to deliver filtered and transformed event streams to users and analysis systems.
- **Data Management**: Improve and deploy distributed storage infrastructure spanning multiple physical sites. Improve inter-site transfer protocols and authorization



DOMA: Intelligent Data Delivery

- In the HL-LHC era, we must deliver more events - and at lower latencies - if the analysts want to make progress!
  - *Low-latency delivery of events requires transformation from long-term archival formats that we want to decrease data size.*
  - *Data should be transformed and delivered at the storage level, not at the workstation.*
  - *Users should be enabled to work on a multitude of data formats (esp. non-ROOT) without having to write them to disk.*
- We are currently prototyping an Intelligent Data Delivery service to:
  - *Extract events from a data lake for fine-grained processing*
  - *Deliver events to analysis facilities at a high data rate.*



IMPACT / Status:

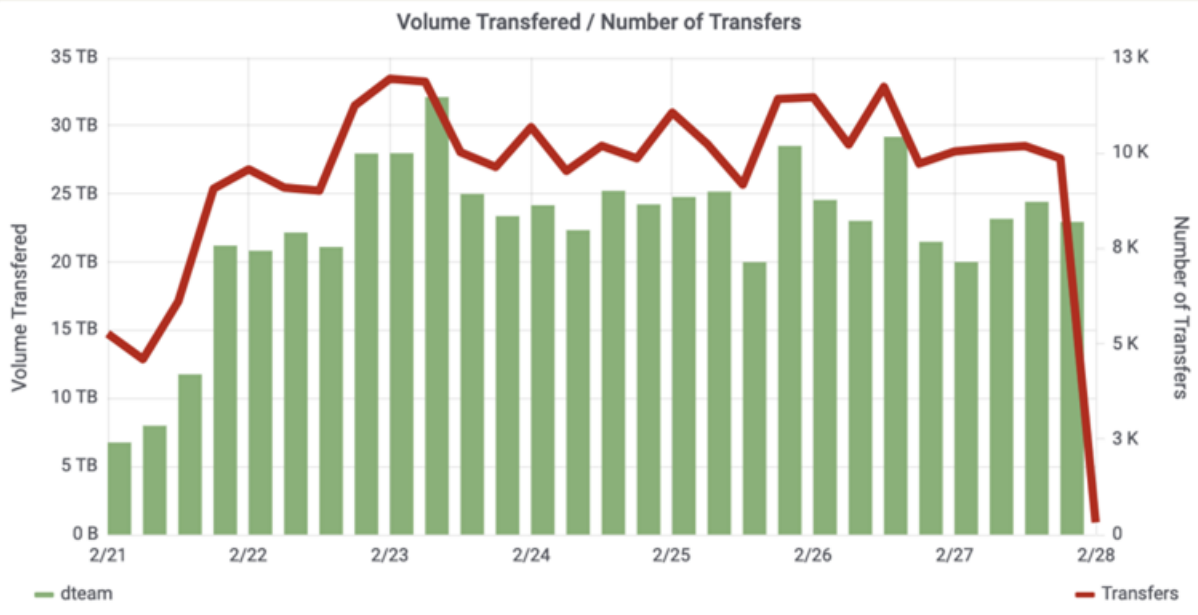
- Working to integrate intelligent data delivery with ATLAS's PanDA for fine-grained processing.
- Can transform and deliver ATLAS xAOD events for analysis.
- Working with Coffea team to deliver CMS NanoAOD events to Jupyter notebooks.

G. Watts (UW/Seattle)

Homepage of the WLCG working group

DOMA: Moving Bulk WLCG Data

- There is a strong movement in the community to move from niche protocols for bulk data movement to more standardized ones such as HTTP.
  - *Bockelman co-leads the working group within the WLCG for "third party copy' (TPC).*
- During IRIS-HEP, HTTP-TPC has gone from small test transfers to scale tests on servers to scale tests in the WLCG DOMA community.
  - ***Demonstrated HTTP's ability to achieve speeds similar to GridFTP on dedicated server hardware.***

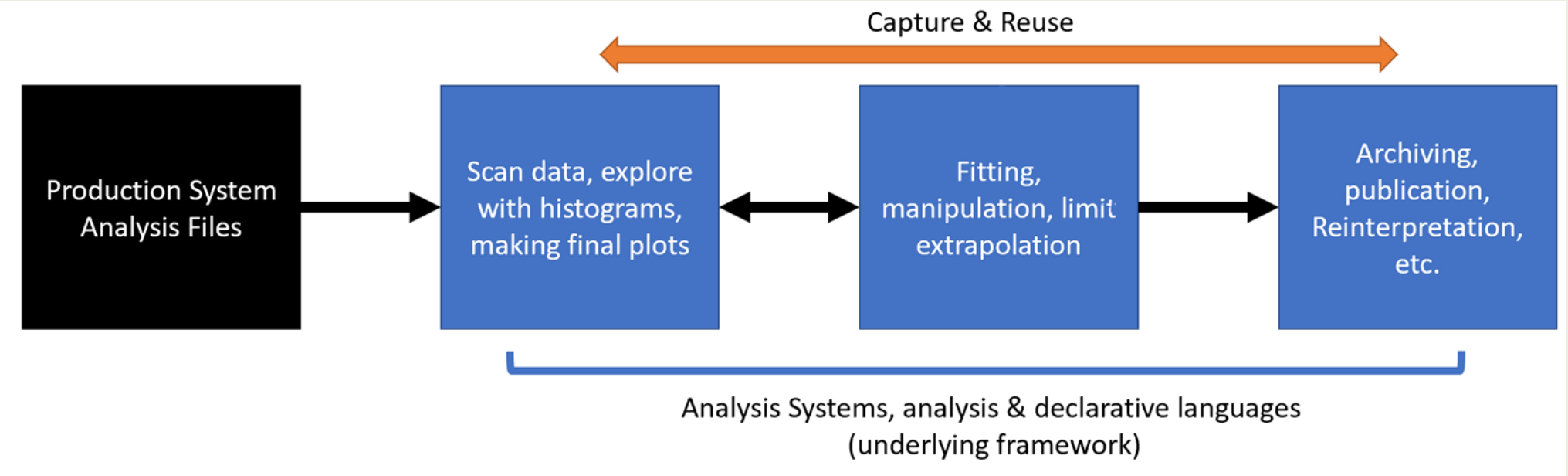


IMPACT / Status:

- Worked to make HTTP-TPC available in the storage systems used by U.S. LHC sites.
- With WLCG, worked to finalize a common, interoperable authorization scheme based on OAuth2 and JWT.

Analysis Systems

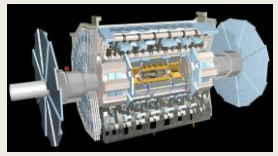
Develop sustainable analysis tools to extend the physics reach of the HL-LHC

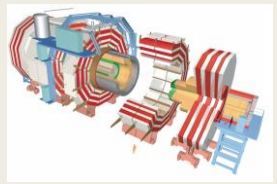


- create greater functionality to enable new techniques,
- reducing time-to-insight and physics,
- lowering the barriers for smaller teams, and
- streamlining analysis preservation, reproducibility, and reuse.

Analysis Systems projects span all stages of end-user analysis.

Analysis Systems - Data Query





Production & Simulation

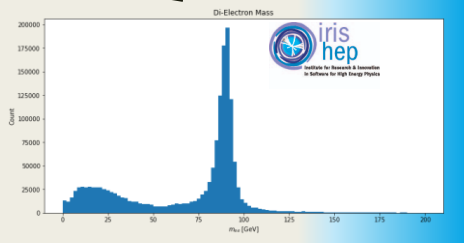
IDDS & ServiceX

Designed for high speed data delivery

Awkward Array

Spark

Coffea



- ServiceX (IDDS) - Collaboration with DOMA to serve analysis data in a “columnar form”.
- Awkward Array - HEP-style column-wise data in the python ecosystem for manipulating the data
- Coffea - column-oriented framework for analysis (developed initially at FNAL in the US CMS context)
    - Builds on top of other backends allowing execution on Spark- or HTCondor-based resources.

Full chain to make a Z mass peak in electron data!

Analysis Systems - Statistical Models

Implementation of widely used statistical tool in modern frameworks

NumPy TensorFlow PyTorch

Installation:

```
$> pip install pyhf
```

By leveraging these tools, we inherit benefits

Auto-Differentiation:

Tensor libraries from ML communty provide exact gradients for use in minimization.

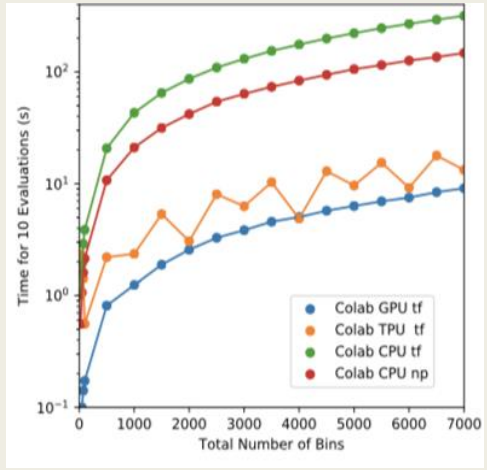
$$\frac{\partial \mathcal{L}}{\partial \mu}, \frac{\partial \mathcal{L}}{\partial \theta_i}$$

Optimizers

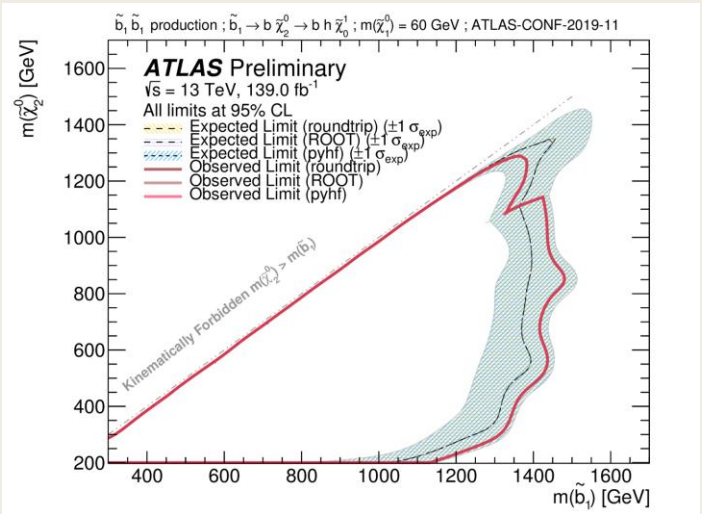
pyhf likeliehood are simple tensor-value python functions. Can use multiple minimization algorithms, such as `scipy.minimize` or MINUIT

Hardware Acceleration

For ML-library tensor backends Computational graph can be transparently placed on hardware accelerators: GPUs and TPUs for order of magnitude speed-up in computation.



Reducing time to insight!



ROOT: 10+ hours
pyhf: < 30 minutes

Preservation & Reinterpretation

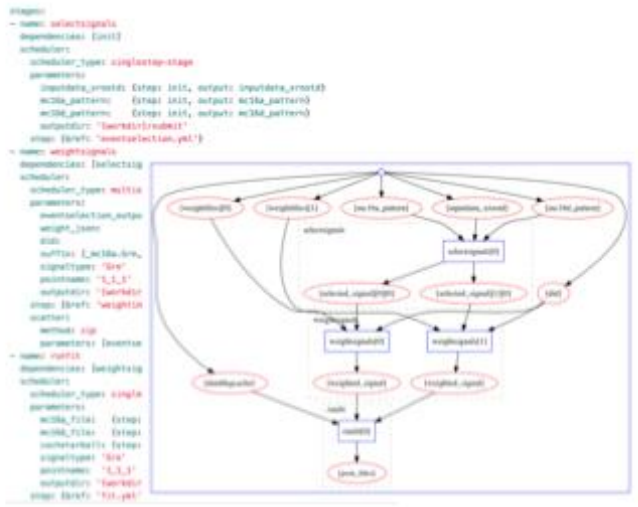
Archiving Real ATLAS Analyses

Using Industry Standard Software Packaging to archive analysis:

- Linux Containers ("Docker")
- Integrated into existing analysis infratructure (revision control, continous intergration, grid computing)

Plain-text JSON formats to capture commands and workflows

Close coordination with CERN Analysis Preservation / Reuse Projects



reana

CERN Analysis Preservation

nature physics

PERSPECTIVE

https://doi.org/10.1038/s41567-018-0342-2

Corrected: Publisher Correction

OPEN

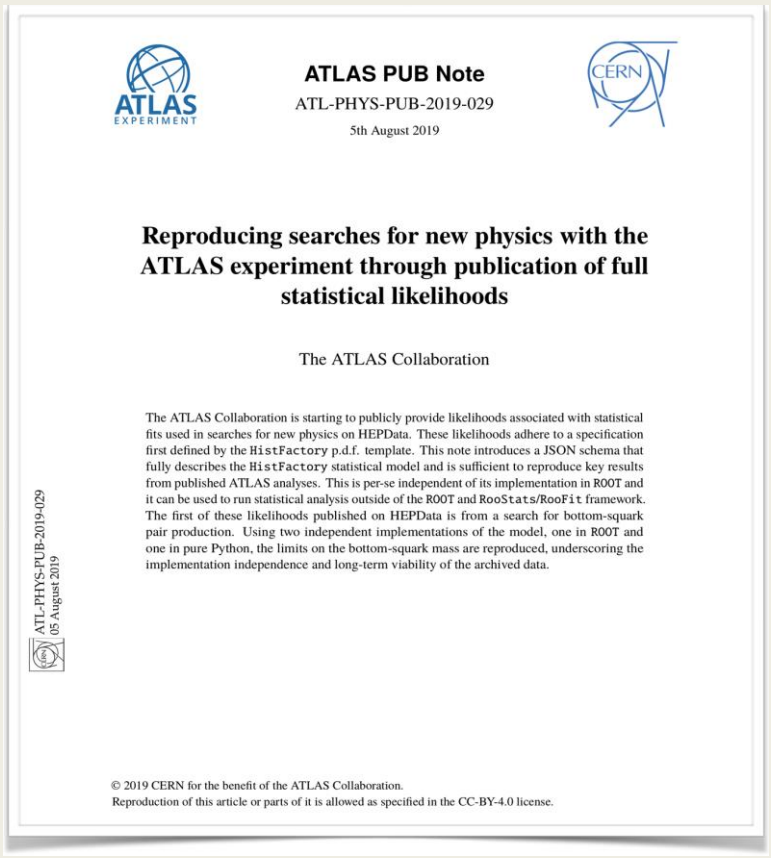
Open is not enough

Xiaoli Chen[1,2], Sünje Dallmeier-Tiessen[1*], Robin Dasler[1,11], Sebastian Feger[1,3], Pamfilos Fokianos[1], Jose Benito Gonzalez[1], Harri Hirvonsalo[1,4,12], Dinos Kousidis[1], Artemis Lavasa[1], Salvatore Mele[1], Diego Rodriguez Rodriguez[1], Tibor Šimko[1*], Tim Smith[1], Ana Trisovic[1,5*], Anna Trzcinska[1], Ioannis Tsanaktsidis[1], Markus Zimmermann[1], Kyle Cranmer[6], Lukas Heinrich[6], Gordon Watts[7], Michael Hildreth[8], Lara Lloret Iglesias[9], Kati Lassila-Perini[4] and Sebastian Neubert[10]

The solutions adopted by the high-energy physics community to foster reproducible research are examples of best practices that could be embraced more widely. This first experience suggests that reproducibility requires going beyond openness.

Preservation & Reinterpretation

First results using the RECAST reinterpretation framework and publishing full statistical likelihoods (using pyhf)



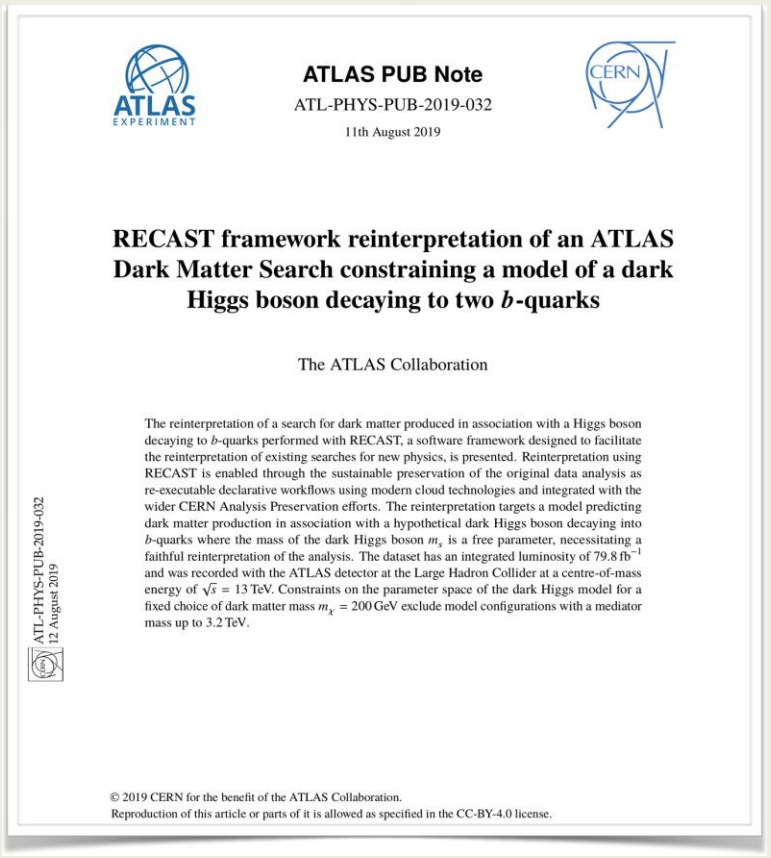
ATLAS PUB Note
ATL-PHYS-PUB-2019-029
5th August 2019

Reproducing searches for new physics with the ATLAS experiment through publication of full statistical likelihoods

The ATLAS Collaboration

The ATLAS Collaboration is starting to publicly provide likelihoods associated with statistical fits used in searches for new physics on HEPData. These likelihoods adhere to a specification first defined by the `HistFactory` p.d.f. template. This note introduces a JSON schema that fully describes the `HistFactory` statistical model and is sufficient to reproduce key results from published ATLAS analyses. This is per-se independent of its implementation in `ROOT` and it can be used to run statistical analysis outside of the `ROOT` and `RooStats/RooFit` framework. The first of these likelihoods published on HEPData is from a search for bottom-squark pair production. Using two independent implementations of the model, one in `ROOT` and one in pure Python, the limits on the bottom-squark mass are reproduced, underscoring the implementation independence and long-term viability of the archived data.

ATL-PHYS-PUB-2019-029
05 August 2019



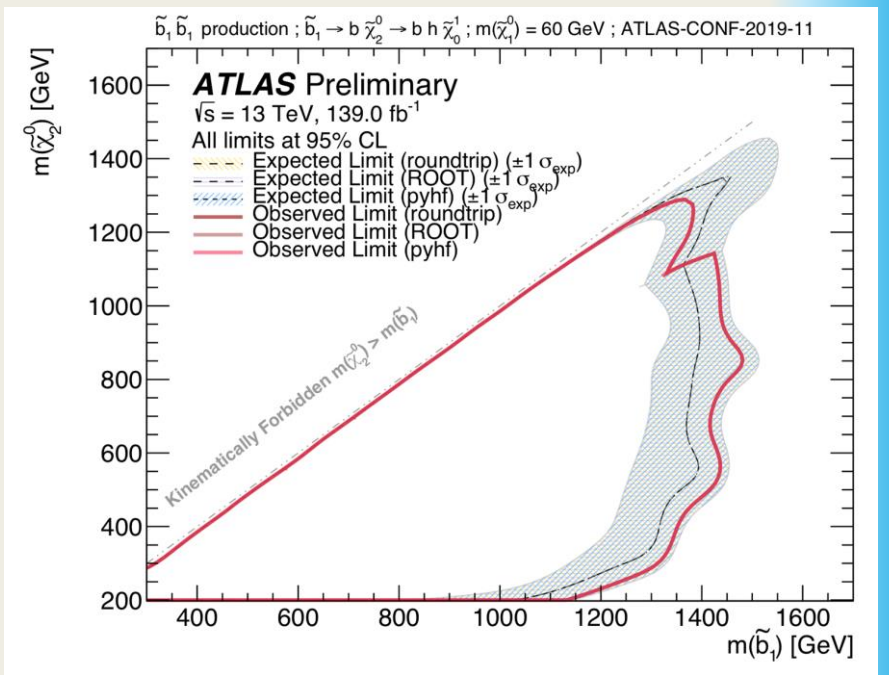
ATLAS PUB Note
ATL-PHYS-PUB-2019-032
11th August 2019

RECAST framework reinterpretation of an ATLAS Dark Matter Search constraining a model of a dark Higgs boson decaying to two *b*-quarks

The ATLAS Collaboration

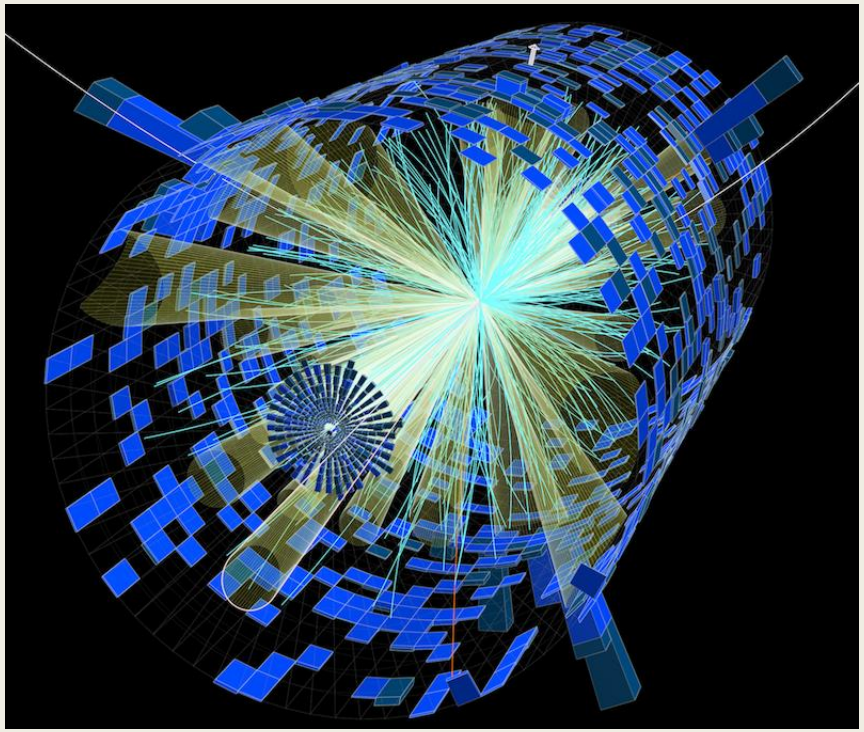
The reinterpretation of a search for dark matter produced in association with a Higgs boson decaying to b-quarks performed with RECAST, a software framework designed to facilitate the reinterpretation of existing searches for new physics, is presented. Reinterpretation using RECAST is enabled through the sustainable preservation of the original data analysis as re-executable declarative workflows using modern cloud technologies and integrated with the wider CERN Analysis Preservation efforts. The reinterpretation targets a model predicting dark matter production in association with a hypothetical dark Higgs boson decaying into b-quarks where the mass of the dark Higgs boson m_s is a free parameter, necessitating a faithful reinterpretation of the analysis. The dataset has an integrated luminosity of 79.8 fb^{-1} and was recorded with the ATLAS detector at the Large Hadron Collider at a centre-of-mass energy of $\sqrt{s}$ = 13 TeV. Constraints on the parameter space of the dark Higgs model for a fixed choice of dark matter mass m_χ = 200 GeV exclude model configurations with a mediator mass up to 3.2 TeV.

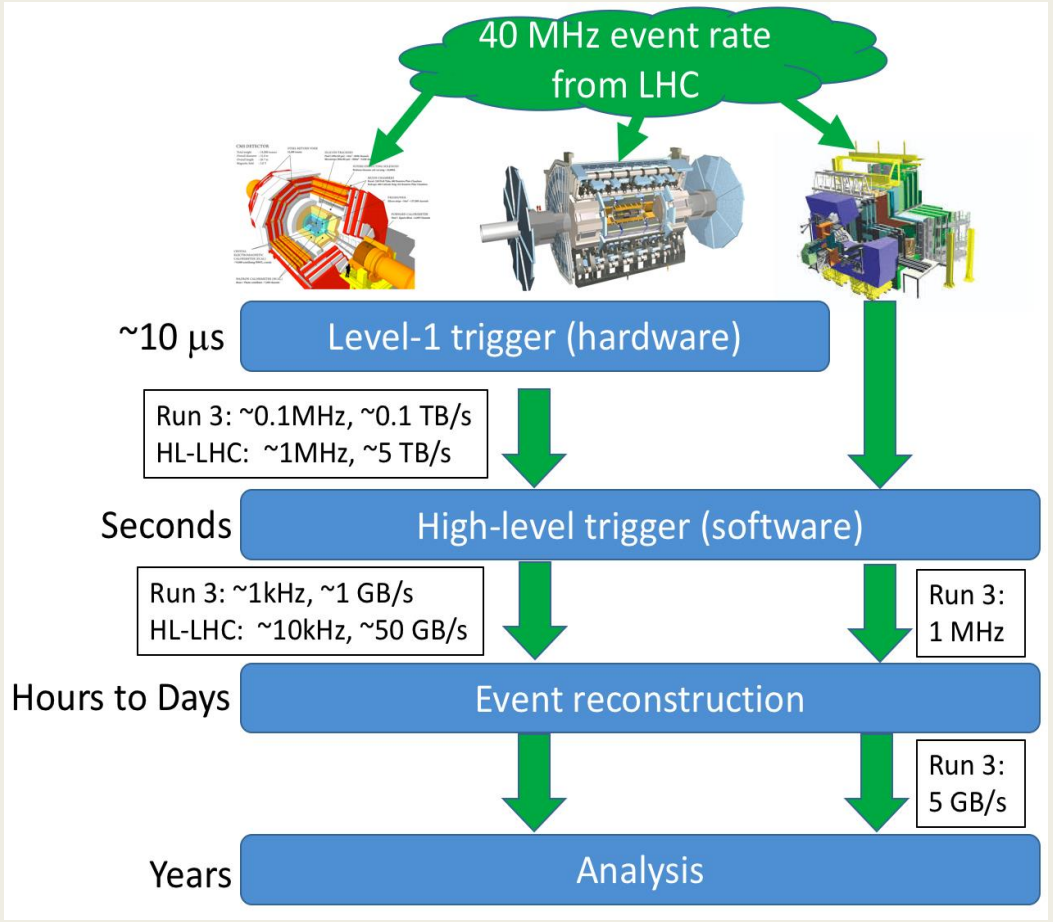
ATL-PHYS-PUB-2019-032
12 August 2019



Innovative Algorithms

Algorithms for real-time processing of detector data in the software trigger and offline reconstruction are critical components of HEP's computing challenge.





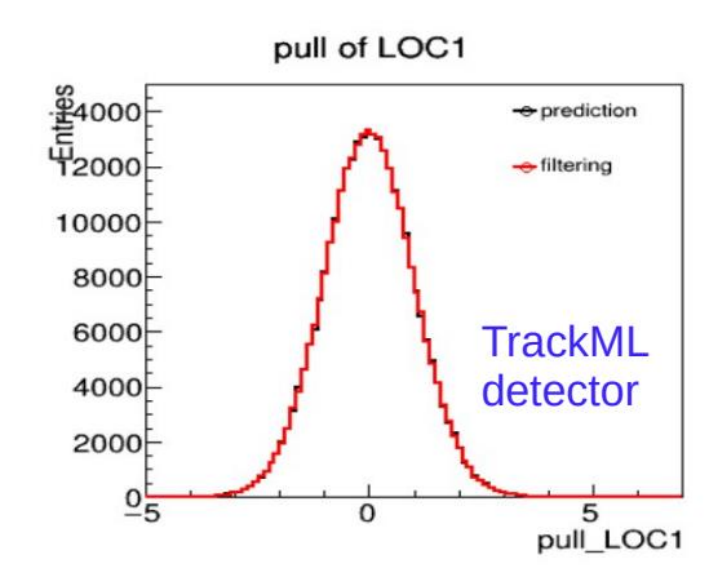
Challenges: pile-up, detector upgrades, emerging compute architectures

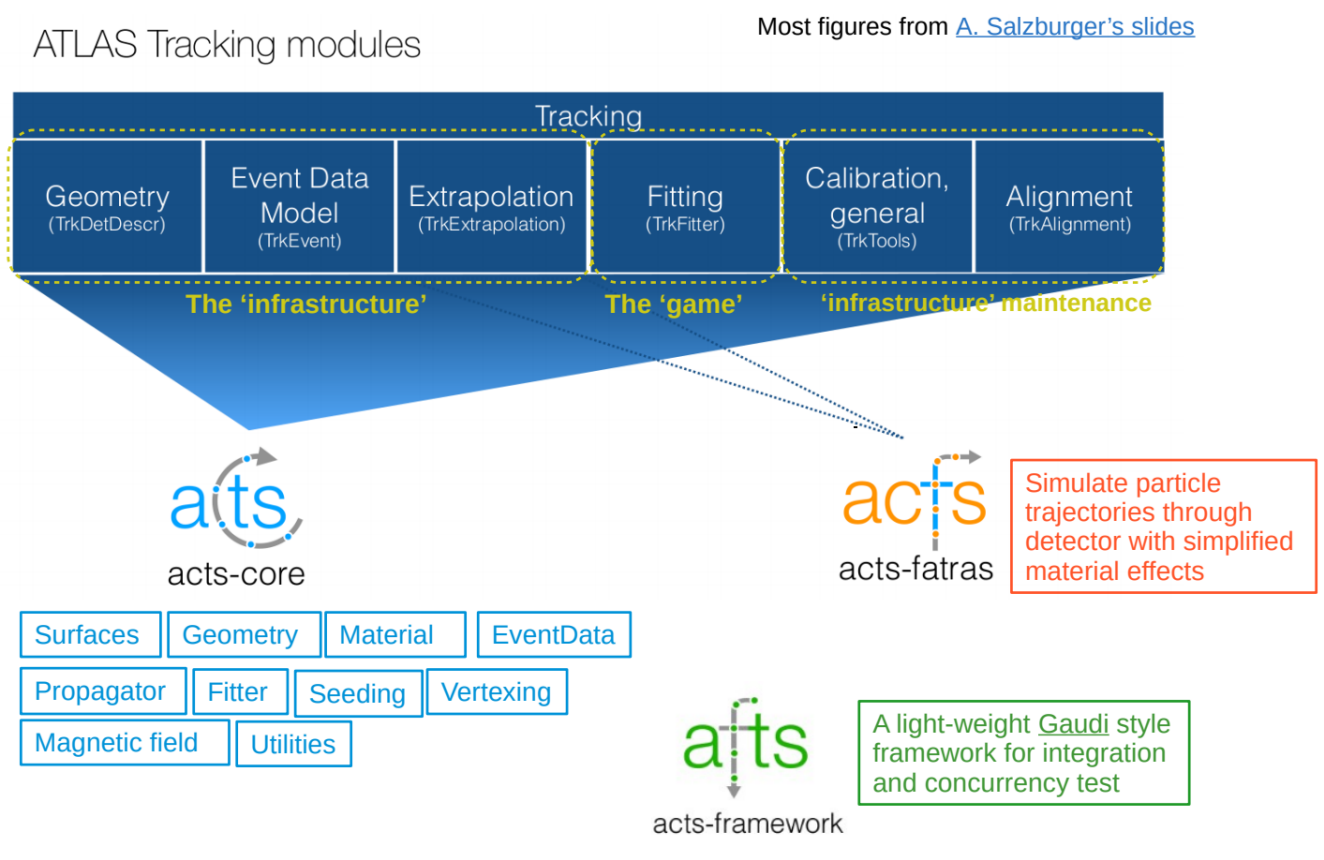
ACTS

"A Common Tracking Software"

Modern, cross-experiment, C++ toolkit for track-finding and more.

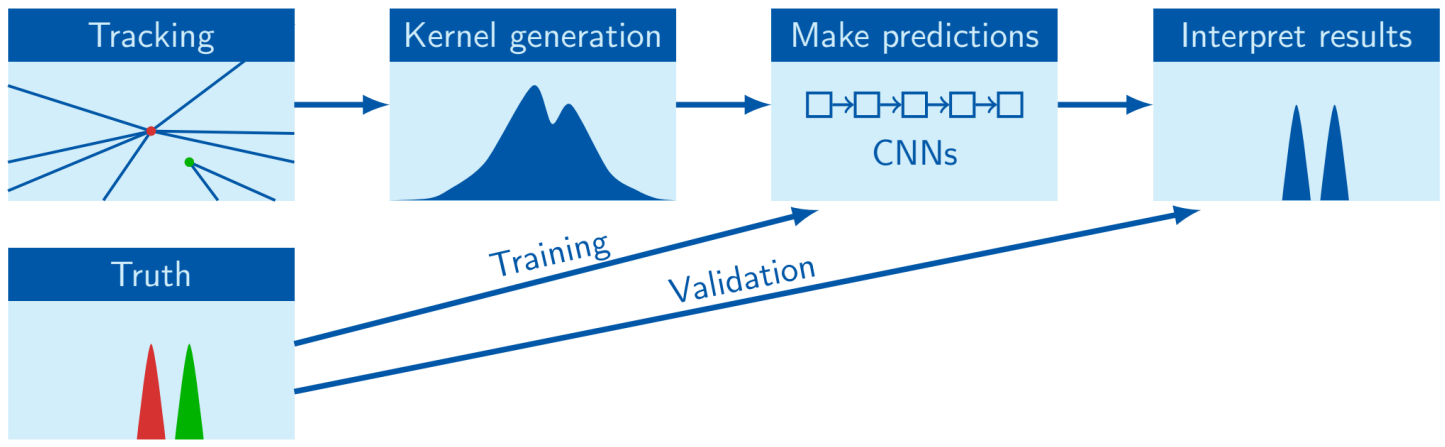
ATLAS, FCC, TrackML Challenge, and links to DD4hep

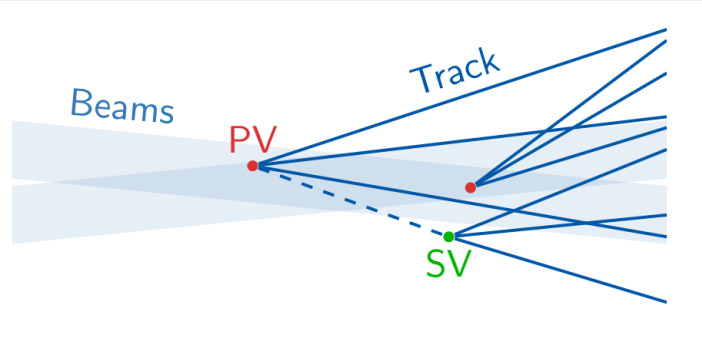




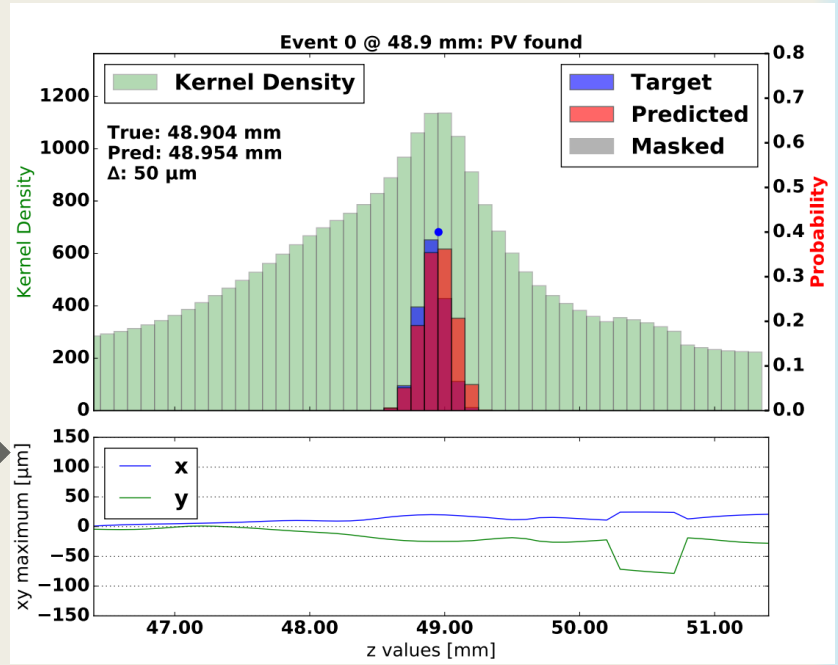
PV Finder

Primary Vertex finding @LHCb using CNN's





Can we do vertexing in a tracker like LHCb using ML?
Proof of Principle has been established
Next: training on large datasets & production in HLT

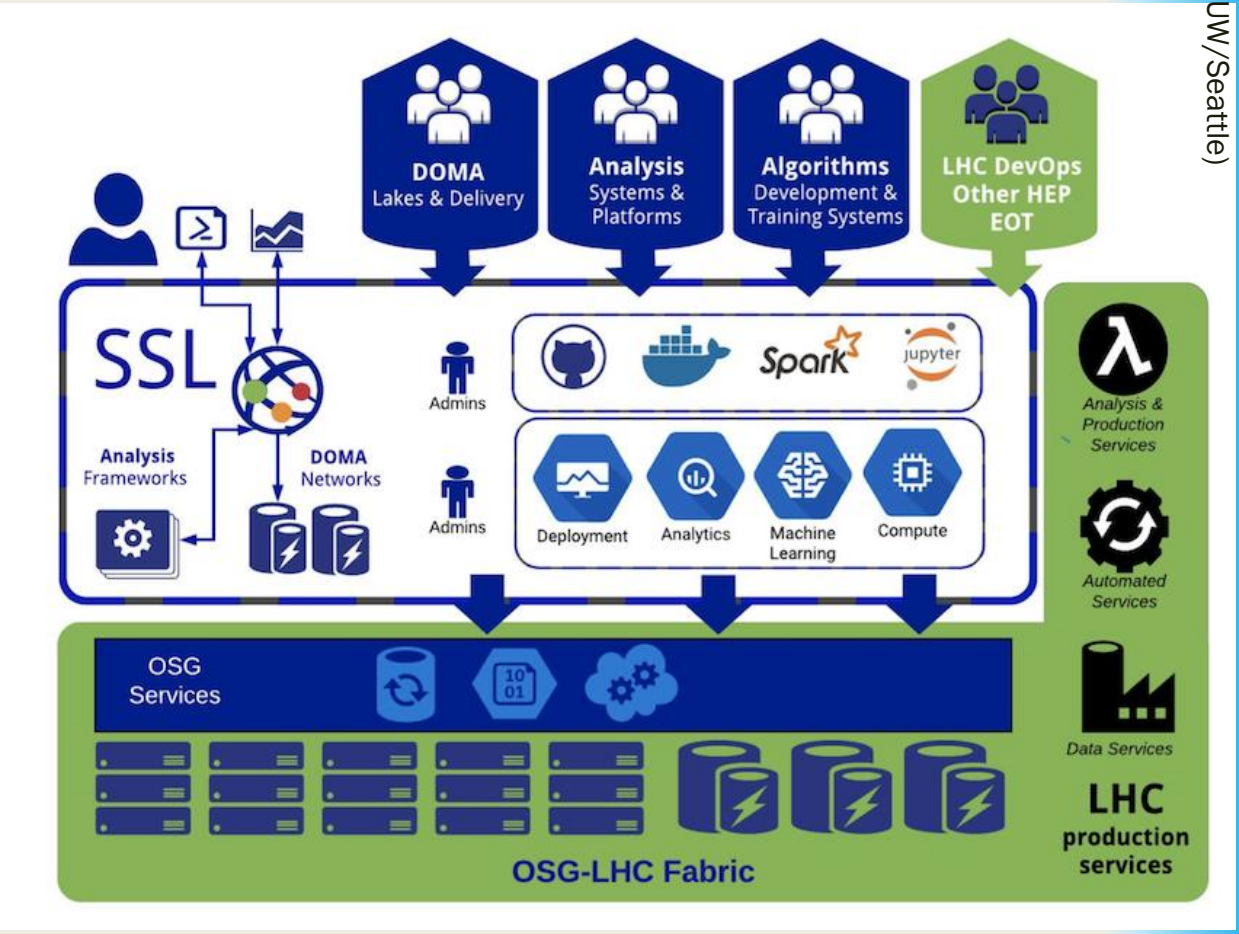


https://gitlab.cern.ch/LHCb-Reco-Dev/pv-finder

Scalable Systems Laboratory (SSL)

Goal: Provide the Institute and the HL-LHC experiments with scalable platforms needed for development in context

- Provides access to infrastructure and environments
- Organizes software and resources for scalability testing
- Does foundational systems R&D on accelerated services
- Provides the integration path to the OSG-LHC production infrastructure



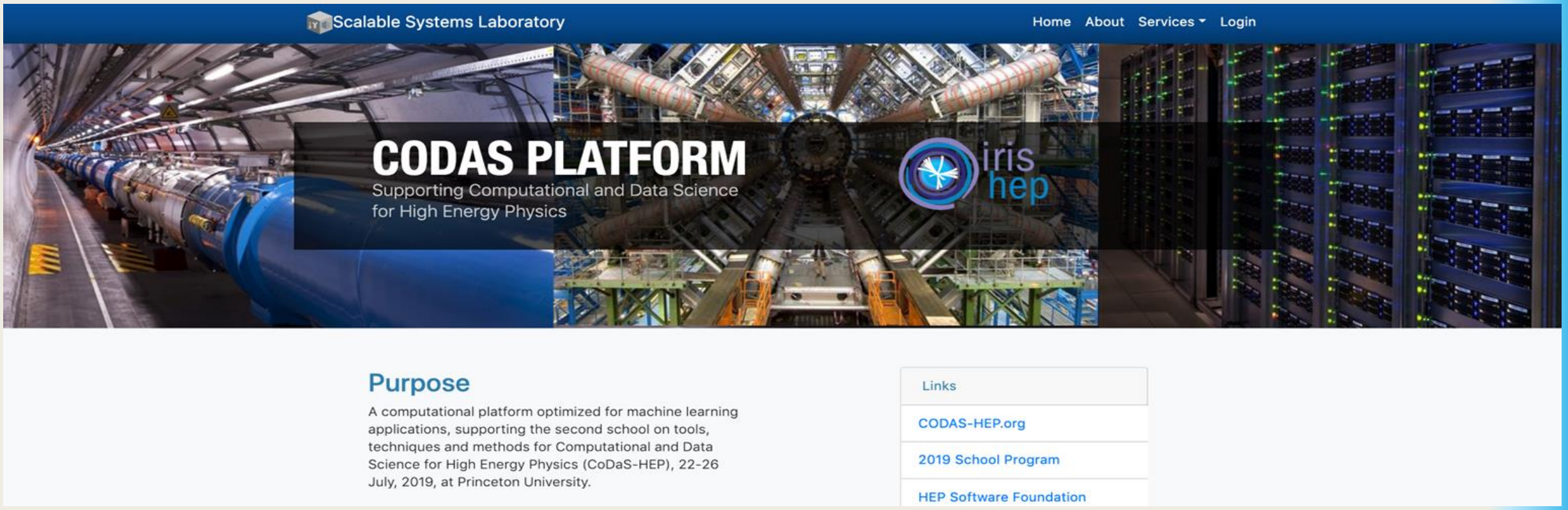
SSL base platform deployed

- Repurposed CS R&D cluster
  - *3k cores, 2x40g to campus 100g SciDMZ; Kubernetes for flexibility for services and compute*
- Deployment of AS & DOMA services (REANA & ServiceX) & ATLAS analytics via SLATE & Helm
- Backfilled by OSG when not in use by IRIS-HEP

Federated ID access (institutional, CERN account), edge services hosting, Unix account provisiong, OSG-LHC sofware environment

SSL Cyberinfrastructure for training

JupyterLab machine learning platform for 55 CODAS-HEP students provisioned by IRIS-HEP SSL Kubernetes hosted services. Leveraged NSF projects: SLATE, Pacific Research Platform, CHASE-CI & LHC Ops.



Open Science Grid (OSG)

- The OSG is a consortium dedicated to the advancement of all of open science via the practice of Distributed High Throughput Computing and the advancement of its state of the art.
- The OSG-LHC group contributes the consortium effort necessary to support OSG.
  - *This effort is roughly ⅓ of the total in OSG today.*
- We focus on shared interests between US ATLAS and US CMS ops programs. These include:
  - Technology & Software
  - Operation of specific services (CVMFS, WLCG accounting)
  - Operational Security
  - Network monitoring
  - *There are other activities in the OSG consortium that serve other broad communities, such as the NSF science and engineering community, DOE-NP, and cosmic and intensity frontier experiments in DOE-HEP.*

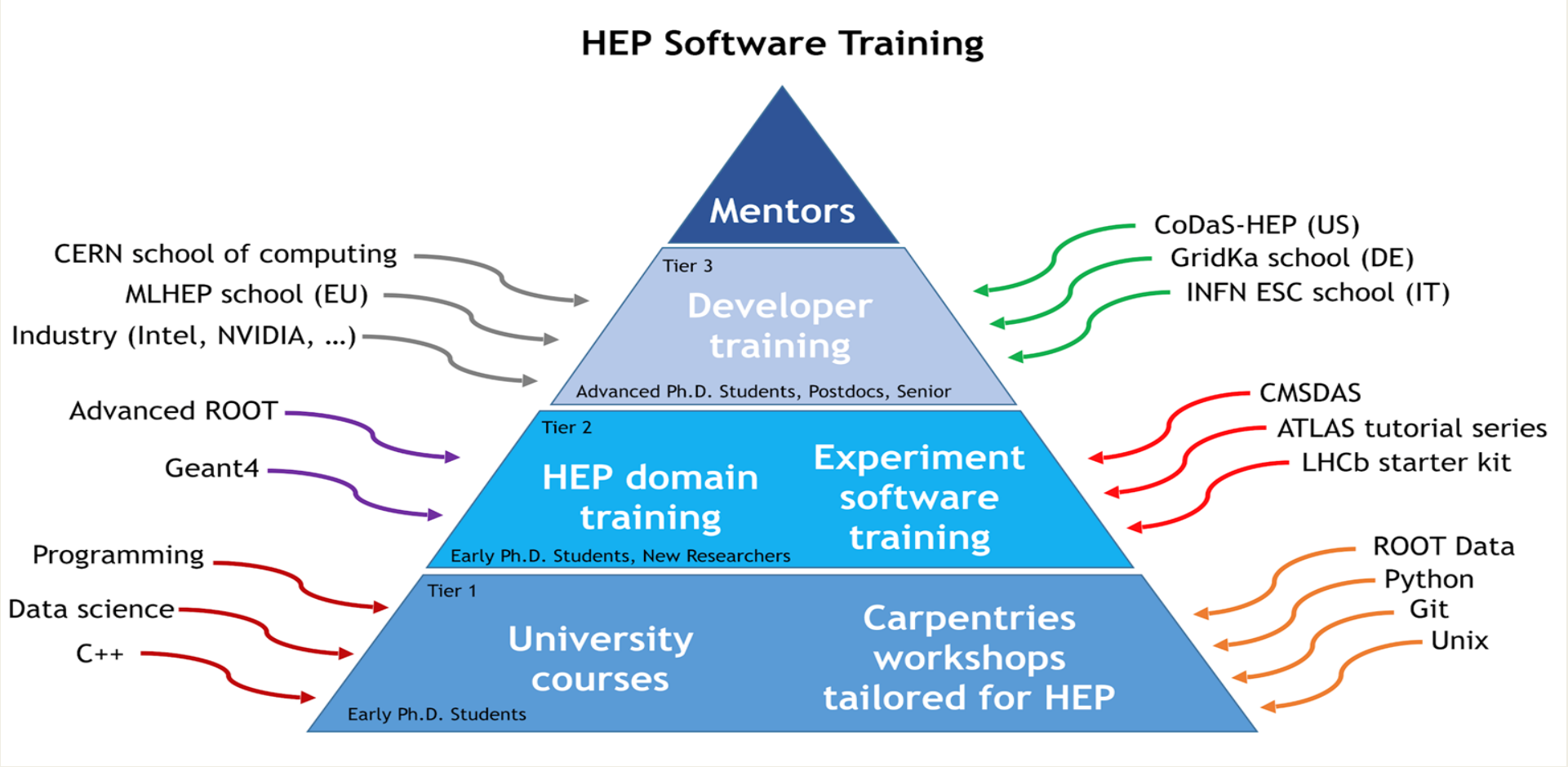
OSG Highlight: Transitioning from GridFTP & GSI to HTTP & Tokens

- Globally, the LHC today depends on GSI for authentication and GridFTP for bulk data transfer.
  - *Neither are supported by their original developers.*
- OSG forked the source code and is maintaining it within the context of community-wide "Grid Community Toolkit" (created for this purpose in 2018).
- We developed a roadmap for replacement of both GSI and GridFTP that has been socialized globally, and across science domains.
  - *August 22nd 2019: Roadmap and schedule presented to LHC ops program via OSG council*
  - *September 12th 2019: Roadmap and schedule presented to WLCG via GDB*
  - *January 2020: First demo of a US-LHC site running services without GSI and GridFTP (prototype / proof-of-concept)*
  - *January 2021: New OSG software release series without GSI and GridFTP.*
  - *January 2022: End of support of GSI and GridFTP in OSG releases.*

OSG-Highlight: Central Service Operations Paradigm

- Traditionally, OSG provided software, testing, deployment & operations documentation/training/support.
  - *Tier-1/2/3 sites instantiated the services for LHC community based on this software.*
- Exploring new paradigm more cleanly separates hardware, infrastructure services, and science support:
  - *Raw hardware capacity is provided by cloud, HPC, Universities & National labs (T1/2/3).*
  - *Centralized service organization(s) deploy & operate services required to turn raw capacity into effective capacity for the US LHC community.*
    - Some services would be run by Ops program, others by entities like OSG (catering across to multiple science domains and HEP frontiers).
  - *Physics support & training*
    - Domain specific projects (e.g. IRIS-HEP & LHC ops program) provide support & training in the tools and software necessary to do the science.
- IRIS-HEP started exploring this new paradigm (collaboration between SSL & OSG):
  - *Support containers in addition to RPMs to instantiate services at T1/2/3*
  - *Developed container security policy document*
  - *Working under leadership of Rob Gardner (SSL/SLATE) & Romain Wartel (CERN) & Jim Basney (TrustedCI) within "WLCG SLATE Security Working Group" to create a new security model that supports this new paradigm.*

Training and Education - Sustainability/Scalability



This is a general framework for training, but from the NSF we have funds from both IRIS-HEP (OAC-183665) and a separate project FIRST-HEP (OAC-1829707, OAC-1829729, http://first-hep.org) which can work towards implementing this model.

CoDaS-HEP 2017

Current IRIS-HEP Fellows

Raghav Kansal
University of California, San Diego

IRIS-HEP Fellow

Jun-Aug 2019

Pratyush (Reik) Das
Institute of Engineering & Management (Kolkata)

IRIS-HEP Fellow
Jun-Sep 2019

ML Hackathon UPRM 2019

CoDaS-HEP 2018

CoDaS-HEP 2019

http://codas-hep.org

IRIS-HEP Community Activities and Events

Upcoming Events:

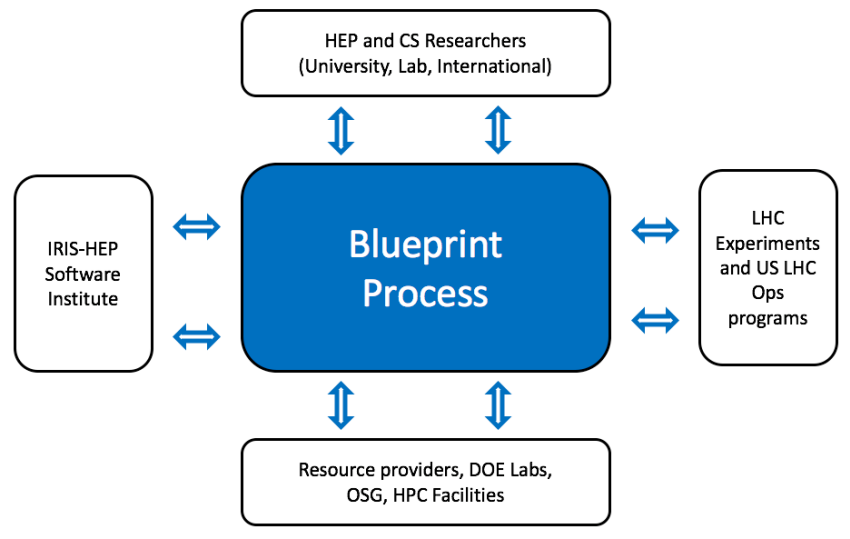
IRIS-HEP team members are involved in organizing the following events:

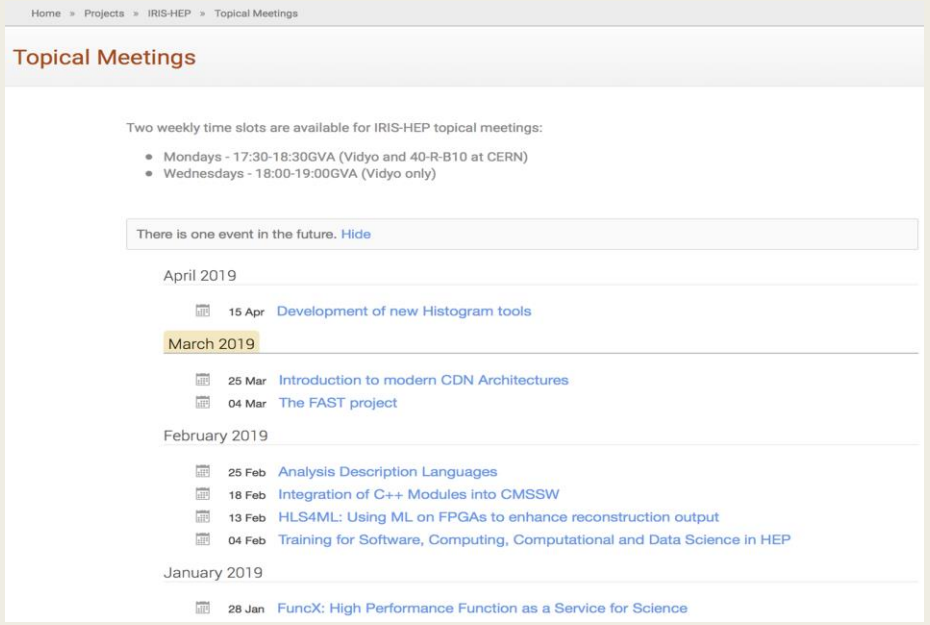
- 29 Jul, 2019 - IRIS-HEP Tutorial: Fast columnar data analysis with data science tools (*Northeastern University / APS DPF 2019*)
- 19 Aug - 23 Aug, 2019 - ATLAS Software Carpentries Training (*LBNL*)
- 10 Sep - 11 Sep, 2019 - Blueprint: Accelerated Machine Learning and Inference (*Fermilab*)
- 23 Oct - 25 Oct, 2019 - Blueprint: A Coordinated Ecosystem for HL-LHC Computing R&D (*Catholic University of America, Washington DC*)
- 13 Dec - 14 Dec, 2019 - Machine Learning and the Physical Sciences at NeurIPS 2019 (*Vancouver Convention Centre*)
- 15 Jan - 17 Jan, 2020 - ML4Jets2020 (in planning) (*New York University*)

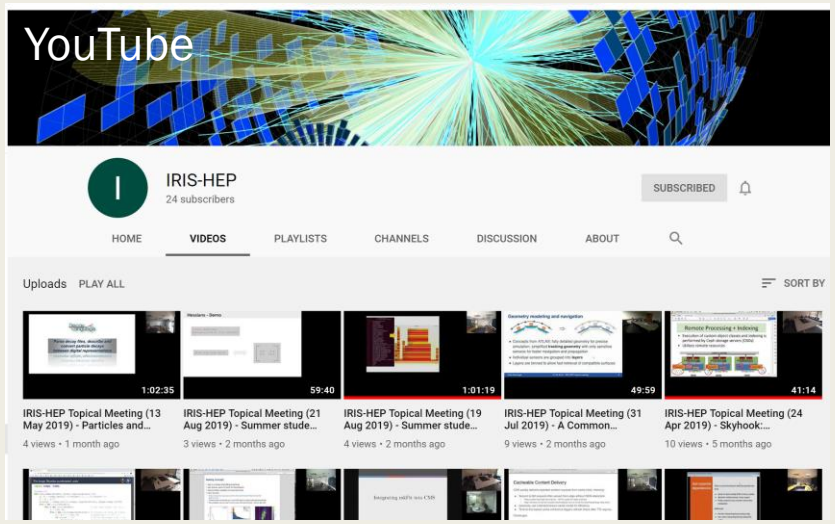
Recent Events:

- 22 Jul - 26 Jul, 2019 - CoDaS-HEP 2019 (*Princeton University*)
- 1 Jul - 2 Jul, 2019 - TrackML Challenge: Grand Finale (*CERN*)
- 21 Jun - 22 Jun, 2019 - Blueprint: Analysis Systems R&D on Scalable Platforms (*NYU*)
- 19 Jun - 20 Jun, 2019 - Analysis Systems Topical Workshop (*NYU*)
- 10 Jun, 2019 - FIRST-HEP/ATLAS Software Training (*Argonne National Lab*)
- 3 Jun - 4 Jun, 2019 - An introduction to programming for STEM teachers (*University of Puerto Rico at Mayaguez*)
- 6 May - 8 May, 2019 - Analysis Description Languages Workshop (*Fermilab*)

Intellectual Hub







Conclusions

- IRIS-HEP has ~28 FTE's working on a large number of CWP topics
  - *Far from covering every topic in the CWP!*
- Focused Research
  - *Analysis Systems, Innovative Algorithms, DOMA*
  - *Infrastructure to move ideas and projects from the lab to the community and production environments.*
- Designed from the ground up to collaborate
  - *With LHC operations programs*
  - *With other funded programs working towards the same goals*
  - *With individuals working towards similar goals*
- For details use our website: http://iris-hep.org.