



# Report from Analysis Ecosystems Workshop II

23–25 May 2022, Paris

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University Nebraska-Lincoln

*Software & Computing round table: Analysis III: Techniques and Tools*  
(<https://indico.jlab.org/event/505/>)

# Hybrid workshop in Paris, IJCLab - 70 participants in person

## Analysis Ecosystems Workshop II

23–25 May 2022  
IJCLab  
Europe/Zurich timezone

Overview

Timetable

Contribution List

My Conference

My Contributions

Registration

Participant List

Videoconference

Code of Conduct

Travel

Accommodation

BoFs and Breakouts

Contact

✉ [hsf-analysis-ecosystems...](mailto:hsf-analysis-ecosystems...)



As part of the search for Beyond the Standard Model physics, an array of next generation particle, nuclear and astroparticle experiments are under construction by global collaborations worldwide. These include the [High-Luminosity Large Hadron Collider \(HL-LHC\)](#) at CERN, the [Deep Underground Neutrino Experiment \(DUNE\)](#) at Fermilab, the [Electron Ion Collider \(EIC\)](#) at Brookhaven National Laboratory, the [Facility for Antiproton and Ion Research](#) at GSI, and many others.

These experiments are massive data generators and the cutting edge data science challenges are significant. For example, the HL-LHC experiments are expected to produce exabytes of science data each year. Discoveries require analyzing these huge data volumes and understanding extremely complex instruments, with ever more sophisticated algorithms. The development of highly performant data analysis systems that reduce "time-to-insight" and maximize physics potential is crucial. This involves the continued innovation by existing community tools like [ROOT](#), new cutting-edge [data science tools](#), the development of dedicated [analysis facilities](#), advanced machine learning and entirely new routes to explore, such as differentiable programming.

## [Workshop Agenda](#)

# Analysis Ecosystems Workshop I



- First analysis ecosystem workshop was organised almost 5 years ago in Amsterdam <https://indico.cern.ch/event/613842/>
- Main idea was to examine the analysis ecosystem, currently and in the future with a 5-10 year view
  - Evolution of ROOT
  - Development of analysis tools landscape
  - Connection to other sciences

## AE1 Development Conclusions

The outcomes of AE1 were summarised in an 11 page [report](#)

- Ascendancy of Python
  - Critical to better connect ROOT to Python (PyROOT support) and the data science ecosystem
- Yet C++ will persist
  - We didn't see any serious competitor at that time on the performance front
- Modularity is important
  - Containers help with isolation from underlying OS
- Decouple what you want from how you get it (declarative/functional)
  - And make sure provenance is saved
- Event throughput is the golden metric
  - But constraints of *latency* for interactive and *event file size* for storage costs

[Introduction to workshop: Graeme A Stewart](#)

# AE2 Topics

Analysis Facilities

ML and Autodiff Workflows

Reduced Formats (nanoAOD, PHYSLITE)

UX and Declarative Languages

Metadata & Systematics

Realtime Trigger Analysis

Dedicated plenary talks

Discussion sessions

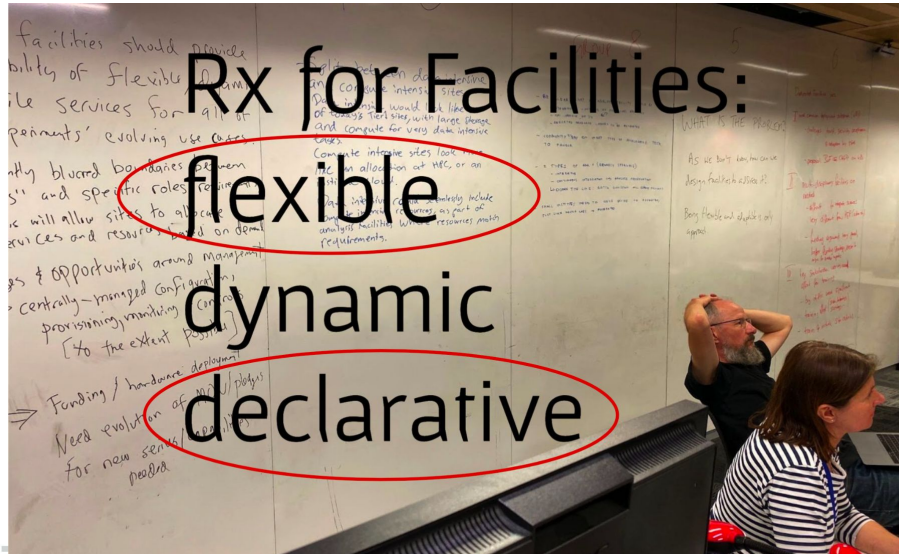
Pickup badges and lunch tickets		
Auditorium Joliot Curie, IJCLab		
08:45 - 09:00		
09:00	<b>Welcome</b>	Michel Jovuin et al.
Auditorium Joliot Curie, IJCLab		
09:00 - 09:15		
	<b>Introduction to the Workshop</b>	Dr Graeme A Stewart
Auditorium Joliot Curie, IJCLab		
09:15 - 09:45		
	<b>New Advances in Analysis Facilities</b>	Robert Gardner
Auditorium Joliot Curie, IJCLab		
09:45 - 10:00		
10:00	<b>Analysis frameworks and Analysis Facilities: user experience</b>	Nick Smith
Auditorium Joliot Curie, IJCLab		
10:00 - 10:15		
	<b>Impact on Analysis Facilities in the context of DOMA evolution</b>	Alessandra Forti
Auditorium Joliot Curie, IJCLab		
10:15 - 10:30		
<b>Coffee Break</b>		
Espace Joliot Curie, IJCLab		
10:30 - 11:00		
11:00	<b>Data Analysis Metadata Review</b>	Thomas Kuhr
Auditorium Joliot Curie, IJCLab		
11:00 - 11:20		
	<b>Big Questions in Systematics Processing</b>	Stephan Hageboeck
Auditorium Joliot Curie, IJCLab		
11:20 - 11:40		
	<b>ML Tooling and Use Landscape in HEP</b>	Sean Joseph Gasiorowski
Auditorium Joliot Curie, IJCLab		
11:40 - 12:00		
12:00	<b>Differentiable Programming in HEP</b>	Lukas Alexander Heinrich
Auditorium Joliot Curie, IJCLab		
12:00 - 12:20		
	<b>Extra Discussion</b>	
Auditorium Joliot Curie, IJCLab		
12:20 - 12:30		

14:00	<b>AFs in CERN</b> Eric Tejedor Salceda	<b>Metadata paper: Discussion of next steps</b> Paul James Laycock	<b>Intro</b> Lukas Alexander Heinrich et al.
	<b>AFs in CMS</b> Lindsey Gray		<b>Generative Model Training &amp; ML Infrastructure</b> Engin Eren
	<b>AFs in ATLAS</b> Alessandra Forti et al.		<b>200-1-101, UCLab</b> 14:10 - 14:30
	<b>AFs in LHCb</b> Dr Nicole Skidmore		<b>Differentiable Design Optimization</b> Giles Chatham Strong
			<b>200-1-101, UCLab</b> 14:10 - 14:30
15:00	<b>Discussion "Bridging analysis frameworks stakeholders and resource providers for future analysis HL-LHC realities"</b> Nicole Skidmore et al.	<b>100-0-A018, UCLab</b> 14:00 - 15:00	<b>Discussion</b> Lukas Alexander Heinrich et al.
	Auditorium Joliot Curie, IJCLab	<b>What analysers want: Infrastructure</b> Enrico Guinaud	<b>200-1-101, UCLab</b> 14:50 - 15:30
	14:40 - 16:00	<b>Systematics discussion</b>	<b>AD beyond Python and ML</b> Vassil Vassilev
		<b>200-0-A018, UCLab</b> 15:20 - 16:00	
16:00			

<b>Coffee</b>		
Auditorium Joliot Curie, IJCLab		
16:30 - 17:00		
17:00	<b>ROOT User Workshop Summary</b>	Axel Naumann
Auditorium Joliot Curie, IJCLab		
17:00 - 17:20		
	<b>Analysis user experience with the Python HEP ecosystem</b>	Jim Pivarski et al.
Auditorium Joliot Curie, IJCLab		
17:20 - 17:40		
	<b>Declarative Languages Overview</b>	Sezen Sekmen
Auditorium Joliot Curie, IJCLab		
17:40 - 18:00		

# Analysis facilities: from design to first prototypes

Amsterdam, 2017



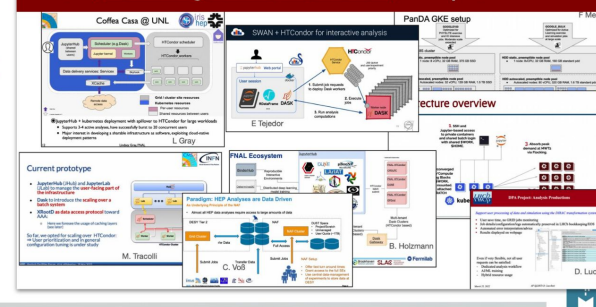
Now

## Now new AFS are materializing

- Facility elements
  - service platform (substrate)
  - clustered storage
  - analysis processing
  - fast WAN for delivery
  - fast LAN for access
  - edge caches
  - interactive services
  - accelerators for ML

**CAPABILITIES:** can I implement new ideas quickly or even interactively? • can I reliably get new results without lots of babysitting? • can I get my data and software to where I need it? • can I share results / grant access with my team worldwide? • can I run on the hardware I need (e.g. train ML models) • can I preserve my analysis / port it to a new facility

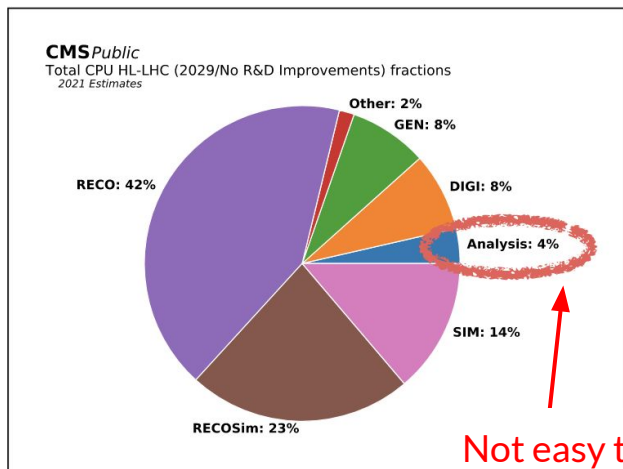
A. Forti, HSF Analysis Facilities Forum, 21-April 22



New Advances in Analysis Facilities - Robert Gardner

# Analysis facilities: from the user PoV

## Analysis Tools and Analysis Facilities: user experience Nick Smith



Not easy to  
quantify  
“Dark” analysis

Focused a lot on fast - it's not the  
bottleneck anymore. Now we have  
to make things easier.

**Fast**

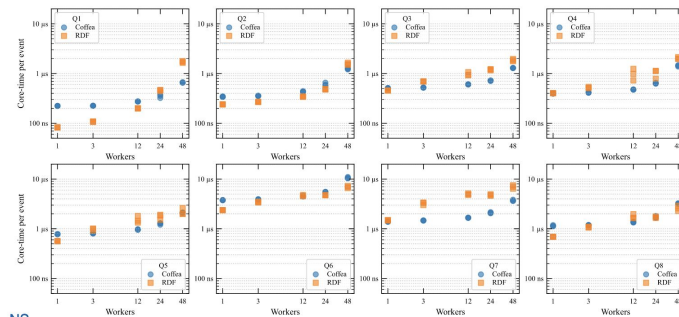
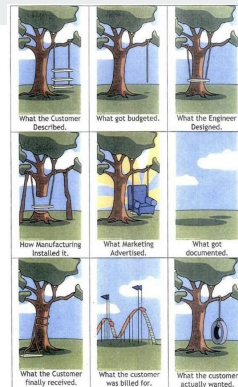
- We're all fast *enough*  
-  $\mu$ s to ms per event

Solutions must be:

**Easy to use**

**Scalable**

**Fast**





# Analysis facilities: what to take into consideration

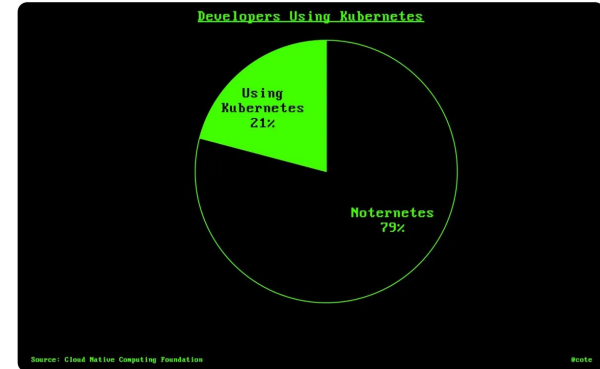
MANCHESTER  
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DOMA Evolution

- HL-LHC scale of data has initiated a revision of this model introducing DOMA activities to look at
  - Network (latency/bandwidth/network orchestration),
  - Caches (hide latency, protect source storages, use diskless sites)
  - Storage QoS (reliability, vs cost vs performance)
  - Storage Deployment and Operation models (full storage, vs caches, vs remote access)
  - Access protocols (gridftp vs https, root, s3)
  - AAI (x509 vs tokens)
  - Storage type (object stores vs posix)
  - Data formats (data transformation and delivery services)
  - Introduction of DataLake and CDN concepts
- So what has all this to do with the Analysis Facilities?
  - AFs use a lot of these concepts to optimise data access for new workflows



3



[Current discussion](#) that Kubernetes has “Crossed the Chasm” and “is entering the mainstream.”

# Highlights from AF discussions



- Early testing is a good approach!
- Need to create the shared knowledge database about DOMA related technologies and its integration in AF (e.g. tokens, xcache)
- Work together with analysis frameworks developers to achieve better user experience
- How to organise possibility for users to share environment
- Importance of easy reproducible installation for Analysis Facilities (!)
- Analysis Grand Challenge could be used as a baseline test for scalability of AF and Data Lakes
- Collection of AF related metrics for better understanding what users are doing on facility
  - Working on analysis performance, resource usage and UX metrics

Lots of topics to be followed up in [HSF Analysis Facilities forum!](#)

# Machine learning: “big” issues

## Large models (that are also big)

This is the **number one advancement of ML in industry, and we're not using it**

- Models trained at scale with many, many parameters are showing a degree of generalisation and performance that wasn't thought possible (particularly for language)

We didn't discuss it much, mostly because we have no experience with this type of thing. -> possible industry collaboration point?

Would require very carefully selected task definition, lots of training data, and a metric buttload of compute



Foundation models in HEP

[ML tools and differentiable computing workflows](#) - Lukas

Alexander Heinrich, Nathan Daniel Simpson

## Big question mark: is it worth it?

How does it compare to existing methods?


- Summary statistic-based methods, e.g. INFERNO, neos, have shown some improvement on toy problems and open data
- Also come with an additional factor of compute, and batching concerns (whole analysis in one batch?)
- Not many other uses with comparisons already done! [that came up today]

Can it scale? *We don't know!*

So one thing that is clear: we need toy problems that have a degree of realism for comparison, along with expert-tuned benchmarks from standard methods

Differentiable programming: what we should expect?

# Machine learning: more tracking of communalities and benchmarking!



## Common, realistic benchmarks!

- Standard ML community has very established problems that are used as metrics for all new methods
  - Handwritten digits (MNIST), CIFAR-10, etc.
- We're taking steps towards making our workflows available to people for this
  - TrackML competition in 2018
  - Calorimeter challenge
  - Your idea here!
- Also could help consolidate training data for large models

## Experiment tracking

Clear that we don't do enough of this (and it's not centralised)

- tools exist, like tensorboard, weights and biases, comet.ml

We could also use this in general for analysis optimisation!

- e.g. seeing how your cutflow opt is doing over time, tracking a bunch of principled metrics along the way

# Machine learning: the need of dedicated facilities!



## Platforms

Again, this is not a centralised thing (some people have their own GPU clusters, some don't)

Some effort at CERN, e.g. [ml.cern.ch](https://ml.cern.ch), which provides a jupyter entrypoint to using GPUs + Kubeflow for sophisticated tracking of training workflows

- Also work on a VSCode frontend

Nice if more effort put into this kind of thing + visibility, especially for people still training on lxplus CPU [they exist, and we should end their suffering]

# User experience and declarative languages: key items to improve

## Pain points in analysis user experience, ordered

### 1. Systematics

- Recurring topic throughout this workshop: this is not solved

### 2. Metadata

- Finding & handling information

### 3. Scale-out

- Prototyping vs scale-out, different implementations / details on different sites
- Need for consistent environments across all resources

# User experience and declarative languages: interoperability!

- Identified **histograms** as key area for improving interoperability
- We should ensure that **Python bindings** are interoperable
- Demand for general **statistical model format** based on JSON
- Discussion about **data interoperability** at the level of individual **columns** (also in memory)



# User experience and declarative languages: some ideas what to improve in future

## Towards a better future - what would we like?

- Automatic (graph-based) **optimization** (à la RDF Vary()) to enable users to focus on physics instead of optimization
- **Grouping of columns into objects** to allow physics reasoning
- **Factoring out** the **analysis chores** to mini-frameworks / libraries
- More **documentation and learning material**

# Reduced data formats:

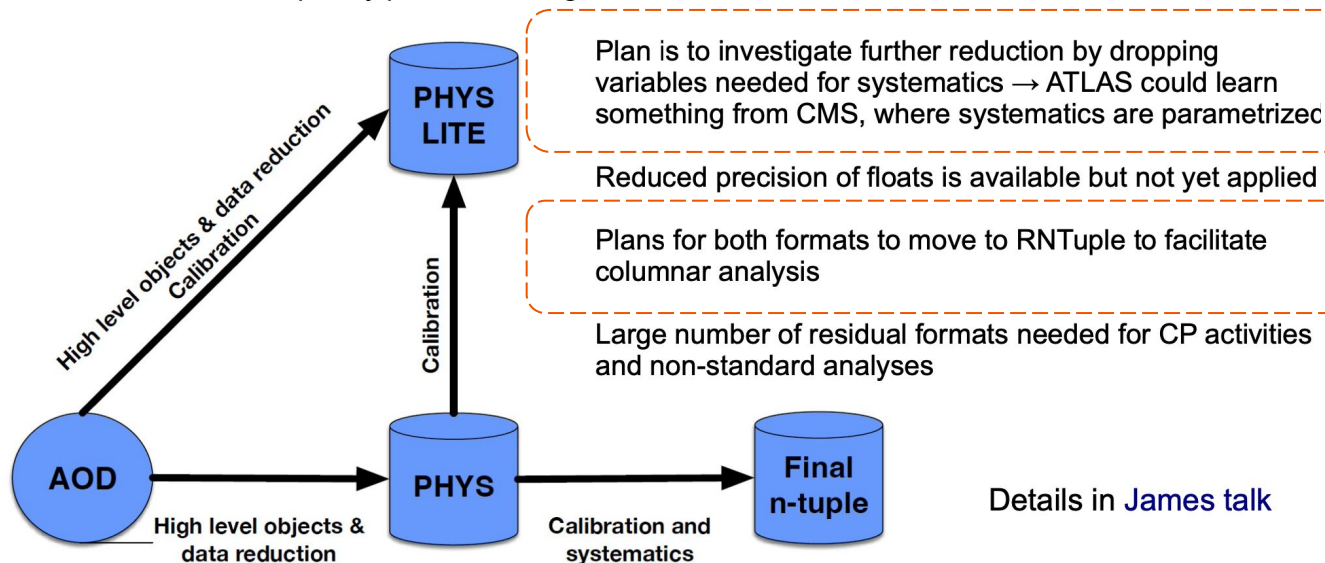
4 / 6

## Reduced Formats in ATLAS

**AOD (300-600 kB/event) → PHYS (30-50 kB/event) → PHYSLITE (10-15 kB/event)**

Common formats aiming to be used by 80% of the analysis (PHYS in run-3, PHYSLITE in run-4)

PHYSLITE will be frequently produced using latest recommendations for calibrations etc.



Details in [James talk](#)

# Reduced data formats:

## Reduced Formats in CMS

3 / 6

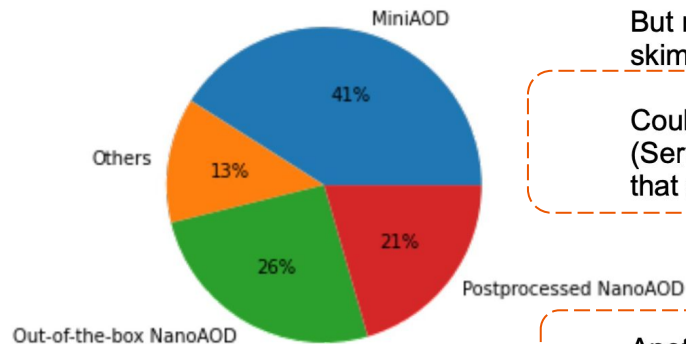
**AOD** (~500 kb/event) → **MiniAOD** (~50 kB/event) → **NanoAOD** (~2 kB/event)

MiniAOD format contains slimmed object collections, PFlow and tracks

NanoAOD is a flat ntuple, strictly controlled to keep size small, containing high-level objects

MiniAOD and NanoAOD serve 85% of all current analysis!

Floats stored with limited precision (based on detector resolution)



But nearly half of NanoAODs are customized (either skimmed or extended with extra info)

Could avoid the „full-copy“ overlaps by central service (ServiceX, Crab, Dask, regular Batch, ...) that allows people to write extra columns („LegoAOD“)

Details in [Lindsays talk](#)

Another possibility: Object stores, eg. to avoid copying columns across processing tiers (→ see talk by [Nick](#))

# Metadata & Systematics



## DAWG - Metadata paper review

John De Stefano (BNL, IT)  
Elizabeth Gallas (Oxford, ATLAS, databases)  
Giacomo Govi (INFN Padova, CMS)  
Thomas Kuhr (LMU Munich, Belle II)  
Igor Mandrichenko (FNAL, IT)  
Tibor Simko (CERN, IT, reusable analyses)

## The Paper

### Constraints on future analysis metadata systems in High Energy Physics

T. J. Khoo<sup>5</sup>, A. Reinsvold Hall<sup>10</sup>, N. Skidmore<sup>16</sup>, S. Alderweireldt<sup>15</sup>, J. Anders<sup>13</sup>, C. Burr<sup>3</sup>, W. Buttinger<sup>9</sup>, P. David<sup>11</sup>, L. Gouskos<sup>3</sup>, L. Gray<sup>4</sup>, S. Hageböck<sup>3</sup>, A. Krasznahorkay<sup>3</sup>, P. Laycock<sup>1</sup>, A. Lister<sup>14</sup>, Z. Marshall<sup>6</sup>, A. B. Meyer<sup>2</sup>, T. Novak<sup>2</sup>, S. Rappoccio<sup>12</sup>, M. Ritter<sup>7</sup>, E. Rodrigues<sup>8</sup>, J. Rumsevicius<sup>3</sup>, L. Sexton-Kennedy<sup>4</sup>, N. Smith<sup>4</sup>, G. A. Stewart<sup>3</sup>, and S. Wertz<sup>11</sup>

<https://arxiv.org/abs/2203.00463>

Request a detailed summary of the panel's opinions (short arXiv doc?)

What next?

## Suggestions for Next Step

- Provide a detailed discussion of use cases
- Describe what problems should be addressed, not what the solution is
- Avoid mixing the discussion of the design of a system and how it is used
- Sharpen metadata scopes definitions
- Derive requirements from use cases, assign them to metadata scopes
- Discuss arguments for or against common solutions (across metadata scopes and experiments)

## What will they do?

Start with use cases

across *all* areas

Covering end-to-end, i.e. conditions, analysis metadata, analysis preservation...

Define metadata scopes mapped to use cases

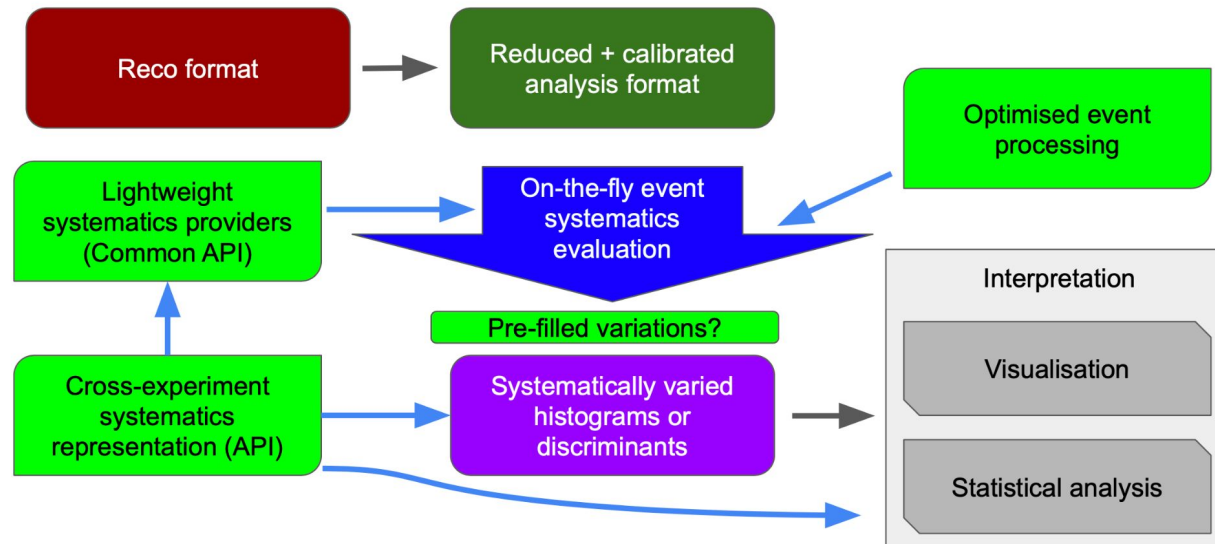
Look for commonality across use cases



Bookkeeping and systematics handling, Paul James Laycock, Teng Jian Khoo

# Metadata & Systematics

## Vision: The deliverables



# Realtime Trigger Analysis

**LHC challenge: too much data for too few resources**

[Intro to RTTA](#)

[Discussion points](#)

[Contributed slides](#)

## **Solution: do analysis in real-time (on the trigger system)**

Shortest possible time to insight!

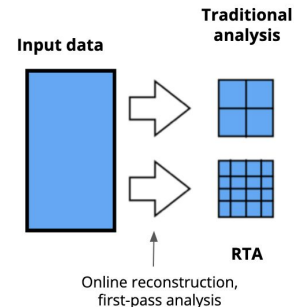
Traditional data analysis is **asynchronous**:

First record and store data, then reconstruct/analyze it



Change of paradigm with quasi-**real-time analysis**:

Reconstruct/analyse data as soon as it is read out  
so that only (**smaller**) final-state information needs to be stored



ALICE: [online reconstruction \(O2\)](#) ATLAS: [Trigger Level Analysis](#) CMS: [Data Scouting](#), LHCb: [Turbo stream](#)

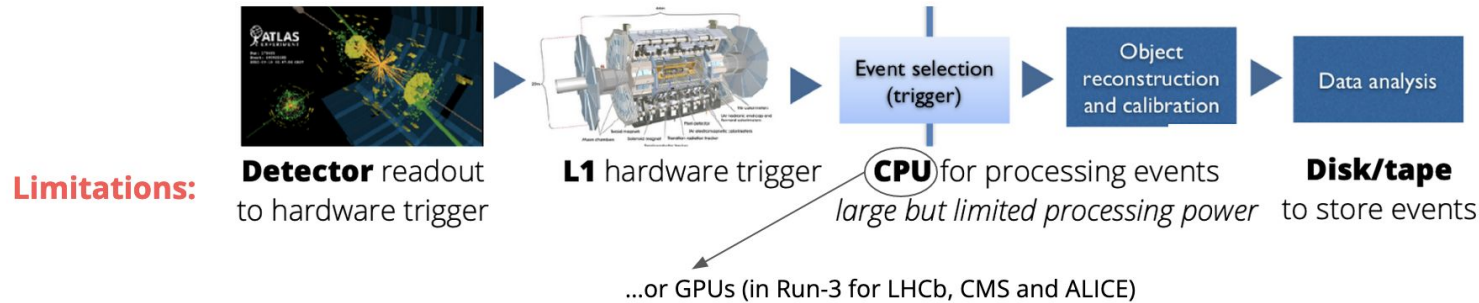
- Event throughput is the golden metric
  - But constraints of *latency* for interactive and *event file size* for storage costs

AE1  
conclusion  
still holds



# Realtime Trigger Analysis

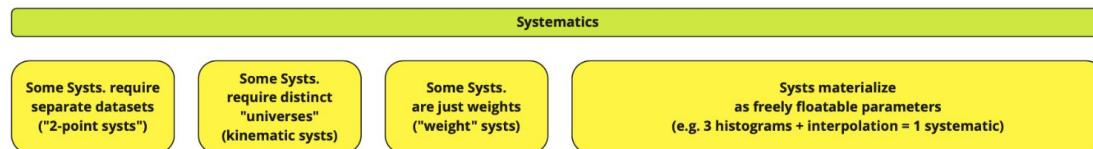
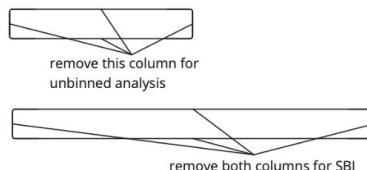
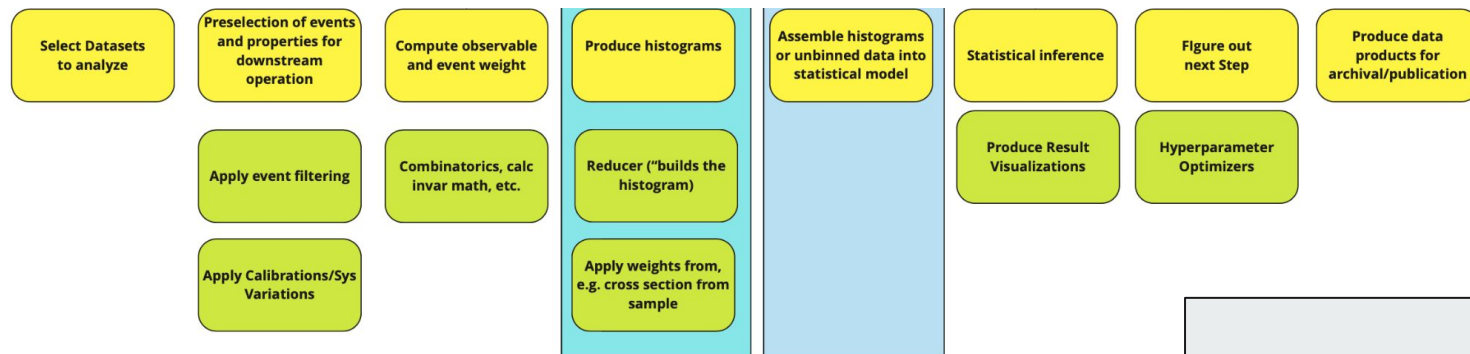
**RTTA → Building analysis ecosystem, on constrained resources**



What kind of analysis ecosystem / analysis facilities  
do we want to build for HL-LHC and beyond?

[Real-Time and Trigger Analysis Overview](#)

# BOF session: Let's Define the Steps of an Analysis Workflow



Could be used for better understanding of "typical" analysis pipeline or for synthetic benchmarks

[Let's Define an Analysis Workflow](#)  
Benjamin Galewsky

# Next steps: community whitepaper



- A lot of time for discussions and a community brainstorming about missing features or future plans!
- As a result, there is an ongoing work about the community report/whitepaper: AE2 Report
  - Main idea is **to document R&D** needed in next 5 years to improve the HEP ecosystem
  - Previous report is available here: <https://zenodo.org/record/6599290>