# LHC Schedule

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<th>Run 1</th>
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<td>Run1: 25 fb⁻¹ usable data at 7-8 TeV</td>
<td>Run2: 140 fb⁻¹ usable data at 13 TeV</td>
<td>Run3: Expect to take ~250 fb⁻¹ of data at 13.6 TeV</td>
<td>Run 4 &amp; beyond: 3-4 ab⁻¹ at 13.6-14 TeV</td>
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<td>Run3: Expect to take ~250 fb⁻¹ of data at 13.6 TeV</td>
<td>10x increase in event rate (trigger upgrade)</td>
<td>~90% of the total LHC dataset</td>
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**Data processing challenges**
- 5-7x increase in luminosity (LHC upgrade)
- 4-5x increase in event size (new detectors)
- 10x increase in event rate (trigger upgrade)

HL-LHC brings unprecedented physics opportunities and computing challenges
Critical for ATLAS physics program that by the start of Run 4 software and computing is ready to:

- process incoming data
- store it with sufficient redundancy
- produce enough simulated MC events
- provide efficient analysis infrastructure

HL-LHC
Run 4 & beyond: 3-4 ab\(^{-1}\) at 13.6-14 TeV
→ ~90% of the total LHC dataset

Data processing challenges
5-7x increase in luminosity (LHC upgrade)
4-5x increase in event size (new detectors)
10x increase in event rate (trigger upgrade)
ATLAS Software & Computing HL-LHC Timeline

**Conceptual Design Report**: HL-LHC Roadmap (Road to Run 4 or R2R4)

**Technical Design Report**: Low level reconstruction (tracking, clustering, object acceptance) - R&D including ML/accelerators and other new techniques & ideas

**Run 4 Feature Freeze**

**Run 4 Performance Freeze**

**Run 4 Release Validated**

**2020**

**2021**

**2022**

**2023**

**2024**

**2025**

**2026**

**2027**

**2028**

**2029**

**2020**

**2021**

**2022**

**2023**

**2024**

**2025**

**2026**

**2027**

**2028**

**2029**

**Ready for HL-LHC data-taking**

**Low level reconstruction**

**High level reconstruction**

**Performance tuning**

**Validation**

**Bug-fixes/contingency**

**ATLAS CDR**

**ATLAS HL-LHC Computing Conceptual Design Report**

**ATLAS Software and Computing HL-LHC Roadmap**

**HL-LHC Roadmap**
Run 4 requires aggressive R&D to stay within budget

Key elements
Fast simulation used for 70% (conservative) or 90% (aggressive) of MC simulation
Faster event generation and reconstruction. Aggressive also means new person power is needed!

There is room for improvement!
Accelerators such as GPUs not considered in this projection, but are expected to play an important role too. Impact of GPUs will be quantified in the TDR.
Key elements

Disk needs mainly arise from storing formats for analysis. Aggressive R&D can reduce disk storage by almost factor 2: common analysis formats, aggressive data compression, increased use of tape, etc…

Tape storage budget has large uncertainties, but huge resources are needed. Tape is required for long-term storage of data and simulation.
Areas of R&D in ATLAS Software & Computing

Database infrastructure, conditions evolution & metadata

ATLAS relies on **large amounts of auxiliary data** (run configuration, calibration & alignment data, data quality, TDAQ, geometries, ...)

Migration of the **conditions database** from COOL to CREST
- Relies more strongly on caches and requires less accesses from Athena grid jobs (1-2 TB per data taking period)

**Other databases** need to evolve to be ready for Run 4: COMA (run database), AMI (ATLAS metadata interface), EventIndex

### Detector description

Current GeoModel service is 20 years old. It needs updates for new detector changes and software improvements

**Run 4 detector** upgrades ([talk](#)) include new Inner Tracker (ITk), new high-granularity timing detector (HGTD), and new muon chambers

Plans are a **unified GeoModel of the whole detector** steered through XML-based database, improved (3D) **visualization** system, several **validation** tools
Areas of R&D in ATLAS Software & Computing

Core software & heterogeneous computing/accelerators

AthenaMT allows the parallel processing of data, while concurrently analyzing multiple parts of an event at the same time (e.g. tracking) — used in Run 3.

Accelerators are a relatively new resource that is not yet widely used, e.g. in production workflows. Ongoing R&D to integrate GPU in Athena.

Dedicated forum HCAF (Heterogeneous Computing and Accelerator Forum) to understand how to efficiently use accelerators — interest in CPU/GPU hybrid workflows.

Decide on technology for algorithm parallelization.

ATLAS Trigger/DAQ exploring FPGA accelerators.

Event generation

MC event generation uses a major fraction of CPU resources.

Theory advances lead to more precise MC including higher order correction which require more resources.

Ongoing R&D

Optimization of settings and choices for the generators and efficient event filtering.

Efficient description of theoretical systematic uncertainties.

Use of HPCs for events with large number of final-state particles.

New generators optimized for GPUs.

New ML methods for event sampling.
Simulation & Digitization

FastCaloSim (FastCalorimeter Simulation) has a long tradition in ATLAS. The calorimeter simulation is most time-consuming part of full simulation (~80% with G4). New fast simulation (AF3) was released an year ago. Includes detailed modeling of the longitudinal and lateral shower evolution to model jet energy substructure. A GAN is used for hadronic shower modelling.

Several ongoing R&D projects are needed for Run 4 FastCaloSim on a GPU (HEP-CCE)

Pile-up effects will be a challenge during HL-LHC. In Run 2, pile-up and hard scatter events were digitized together. In the new MC+MC Overlay used in Run 3 pile-up samples are digitized separately and then overlayed onto the hard scatter. Real data from zero-bias trigger can be used for direct overlay to the digitized simulation.

For Run 4, another idea is track overlay where pile-up tracks are merged after reconstruction. Works well for topologies where hard scatter track reconstruction is not affected by PU.
Areas of R&D in ATLAS Software & Computing

Reconstruction

Object reconstruction very challenging with 200 pile-up interactions on average per event

\[ \mu_{2010} \approx 5 \]
\[ \mu_{2018} \approx 40 \]
\[ \mu_{2029} \approx 200 \]

New & smarter algorithms to handle harsh conditions and benefit from new detectors

Fast track reconstruction ([link](#)) prototype showing large CPU gains possible

ACTS (A Common Track Reconstruction Software): experiment-independent project to achieve CPU reduction and great performance for tracking and also particle flow, supports multi-threading ([link](#))

Integration in ATLAS progressing — already used for vertex finding

IRIS-HEP contributions have been crucial for the success of ACTS!

GNN4ITK (Exa.TrkX in the US) — Tracking using a GNN pipeline on ITk ([link](#))

traccc: Demonstrator of tracking chain on accelerators

Developments ongoing in other areas of reconstruction beyond tracking

GPU-based implementations of calorimeter clustering are about to be integrated & validated
Overview of R&D Projects — Distributed Computing

Distributed Computing

Grid resources and software infrastructure for data management, workflow management, production system, monitoring, analytics, etc…

Data processing relies on distributed resources. ATLAS distributed computing infrastructure need to evolve for HL-LHC (scalability and efficiency)

Ongoing R&D
Token-based authentication
Increase network bandwidth
Integrate new resources, such as HPCs and cloud infrastructure

ATLAS workflows and data management system need to be adapted to serve a variety of HPC platforms

Refinement of fully containerized workflows: all the software in a single container deployed at the HPC site

New schedulers for heterogeneous architectures to use most appropriate resources and balance loads — Raythena, HPX

(Illustration: B. Stanislaus)
Distributed Computing

iDDS and Data Carousel
Intelligent Data Delivery Service (iDDS) is a service to orchestrate the workload and data management systems to transform and deliver data needed to consumers while seeking be efficient in the use of storage, network and processing resources.

Data is stored in the lowest-cost media available (tape) and processing is executed by staging and promptly processing slices of inputs onto faster storage (disk), such that only the minimum required input data are available at any time.

Data carousel is already used for AOD storage in run-3 (link).

Plans for HL-LHC
Reconstructed data stored primarily on tape (with only very partial disk replicas), processed with the Data Carousel.

iDDS provides streaming services for data delivery for an increasing range of complex workflows, such as AI/ML — service for is in production, used for HPO AF3 FastCaloGAN, available for analysis & software teams.

IRIS-HEP contributions have been crucial for the success of iDDS!
Areas of R&D in ATLAS Software & Computing

**DAOD_PHYSLITE:** future common **format for fast analysis**, unskimmed, contains calibrated objects. Small size: ~10 kB/event, total ~1PB/year, to be used by ~80% of all physics analysis in Run 4

**Key concepts for DAOD_PHYSLITE**

RDataFrame and RNtuple in ROOT 7

Columnar analysis and simplified systematics

Lossy compression

**Dedicated computing resources** for more complex end-user analysis workflows such as training complex ML algorithms, exploiting python-based ecosystems for vectorized computations, visualizations etc

Several R&D projects ongoing to identify new tools: scalable Jupyter notebooks, new data delivery services, etc…

Analysis facilities, focus on **interactivity, usability, user-support**, with federated access, store the data and MC samples needed, can provide GPUs and specialized software (e.g. ML), deployed in various forms, for example integrated in large computing centers, as HPCs, or on the cloud

**Several analysis tools developed with IRIS-HEP participation!**
Education, Training & Workforce Development

**Education & training** in software & computing is **critical** to prepare the next generation of scientists — analysts at most levels will need **new skills** to handle increasing datasets.

R&D projects are an exciting opportunity to **engage young scientists and develop careers** — also creates a pipeline of software and computing professionals for operations etc.

Several training initiatives in US ATLAS and ATLAS — **some events organized with IRIS-HEP participation!**

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A priority for the future is training current users on new tools — important for widespread use.

Communities such as IRIS-HEP can make increasing contributions to training infrastructure, curriculum development and interfacing with experiment-specific tools.
ATLAS R&D Demonstrators

Demonstrators planned in next year

proof-of-concept demonstrations to estimate the impact of R&D projects on hardware resources

- e.g. CPU time, GPU time, RAM, disk, tape & network

work ongoing to define configurations, datasets & platforms for these impact studies

Key process for all R&D developments to participate in!

R&D including ML/accelerators and other new techniques & ideas

Ready for HL-LHC data-taking

Project Life Cycle

- Conceptual Design Report
- HL-LHC Roadmap (Road to Run 4 or R2R4)
- Technical Design Report
- Run 4 Feature Freeze
- Run 4 Performance Freeze
- Run 4 Release Validated

R&D including ML/accelerators and other new techniques & ideas

Our calls have been good so far!
Integration in ATLAS Operations

Integration in operations

Mature R&D developments shown to have significant impact need to be integrated with the rest of the software & computing operations. Focus on experiment specific needs and optimizations for ATLAS. Concern about long term support for several community projects.

Long term integration and support through operations is key to sustainable projects.
Improving Synergy with Operations

- Several US-funded R&D projects **key to bridging the resource gap** for the HL-LHC
  - Projects like OSG-LHC, ACTS, iDDS have already made valuable contributions to ATLAS

- Key questions to the **successful transition of R&D to operations**
  - Does the R&D provide **significant gain** & is crucial?
    - Key to participate in demonstrator process — Prototype systems deployed by TDR (2024)
  - What is needed for R&D developments to be **integrated** in the ATLAS **infrastructure**?
    - Early integration to understand scope of work — play active role in organizing development and integration
  - Will there be **adequate maintenance** throughout the lifetime of ATLAS?
    - Embed new projects in experiments soon to increase participation
      - need beginning-to-end systems (full featured prototypes) for experiments in Run 3
Improving Synergy with Operations — Analysis

- **Key goal** is to **integrate new ideas for analysis in the current ATLAS analysis model**
  - Several of the ideas developed in US-funded R&D projects could be integrated in the ATLAS ROOT-based infrastructure — some already are!
  - Topics such as data formats (PHYSLITE, …) are experiment specific, but topics such as transformations to columnar formats & tools to handle systematic variations are possible joint projects.

- **Development of Analysis Facilities considering the ATLAS event and analysis model**
  - Workflows consider the particular way ATLAS deals with data access, handling, calibration & description of experimental uncertainties.
  - Integration of new data analysis and management tools (coffea-casa, serviceX, etc) may require significant dedicated effort to enable widespread use in ATLAS.
Summary & Outlook

- HL-LHC brings unprecedented physics opportunities and computing challenges
- ATLAS is greatly benefitting from collaboration in common software and computing projects
  - Enables sharing ideas, effort and expertise across HEP experiments and with colleagues from other science communities
  - Several projects with participation from programs such as IRIS-HEP have been key to success!
- Many exciting R&D projects ongoing, impact will become clear in the next few years
  - The focus in 2023 will be to demonstrate R&D projects, evaluate their impact on resources and effort
  - Down-selection of R&D projects will lead to the TDR in 2024, which serves as a blueprint for the future
Thank you!

All mistakes are mine
Thanks to contributions from
Alessandro Di Girolamo & Zach Marshall
Rob Gardner, Gordon Watts, Heather Gray, Mike Hance
and others I forgot to write down
Fractions similar for both scenarios, but aggressive R&D can reduce disk storage by almost factor 2
Resource modeling: CPU Projections

**ATLAS Preliminary**
2022 Computing Model - CPU: 2031, Conservative R&D
Tot: 33.8 MHS06*y

- Data Proc: 7%
- MC-Full(Sim): 24%
- MC-Full(Rec): 8%
- MC-Fast(Sim): 7%
- MC-Fast(Rec): 11%
- EvGen: 17%
- Heavy Ions: 8%
- Data Deriv: 8%
- MC Deriv: 6%
- Analysis: 17%

Good mix, but still dominated by FullSim fraction (24%) and EvGen production (17%)

**ATLAS Preliminary**
2022 Computing Model - CPU: 2031, Aggressive R&D
Tot: 16.6 MHS06*y

- Data Proc: 12%
- MC-Full(Sim): 9%
- MC-Full(Rec): 11%
- MC-Fast(Sim): 10%
- MC-Fast(Rec): 7%
- EvGen: 12%
- Heavy Ions: 7%
- Data Deriv: 7%
- MC Deriv: 6%
- Analysis: 6%

About a factor 2 overall speed-up
FullSim fraction significantly reduced
EvGen production now dominates the CPU
Intelligent Data Delivery Service (iDDS)

• iDDS is an experiment-agnostic add-on to PanDA or other workload manager supporting granular data delivery and **orchestration of complex workflows** that are efficient in their use of storage, network and processing resources
  - A joint project with IRIS-HEP, project hosted by HSF
  - Used by ATLAS, Rubin, sPHENIX

• Used in a growing list of applications important for HL-LHC readiness and serving/scaling analysis
  - **ATLAS Data Carousel** processes tape-resident data using a small disk storage footprint via a sliding window orchestrated by PanDA, iDDS and Rucio
    - In production for almost 2 years, reducing the storage needs of analysis object data, the dominant storage load for HL-LHC
    - Ongoing R&D to reduce the footprint and improve performance
  - **Highly scalable ML services**
    - Enable analysts to run processing-intensive AI/ML applications on large scale, geographically distributed, heterogeneous resources
    - Shorten optimization and training latencies by orders of magnitude
  - **Active learning services** drawing on the ML work
Distributed, scalable ML services

Hyperparameter optimization with PanDA/iDDS

Leveraging a variety of distributed platforms in a coherent way for intensive AI/ML processing
Applying ML services via active learning in analysis

- The hyperparameter optimization (HPO) service we developed is in production use for FastCaloGAN, part of the production ATLAS fast simulation AtlFast3
- In working with the analysis community to find the next large scale application of the HPO service, what emerged was active learning, algorithmically a close relative
- The active learning technique we’re using was developed by our ATLAS NYU colleagues
  - In calculating an iso-contour surface \( f(x) \), conventional approach uses a grid with a sampling density not informed by the unknown \( f(x) \)
  - Instead, use an iterative approach, using information about \( f(x) \) from previous evaluation cycles to sample parameter space more efficiently
  - Find an iterative algorithm that suggests points to evaluate that help the most in finding the contour
  - Kyle and colleagues found a computationally efficient one
- In response to interest from analyzers (in particular that team), we adapted our ML hyperparameter optimization service to serve this similar iterative refinement algorithm
- The entire workflow from event generation -> simulation -> reconstruction -> derivation -> limit setting analysis and its iterative refinement loop is implemented and automated using PanDA and IDDS
  - It employs grid and REANA (Reproducible Research Data Analysis Platform) processing resources
- Modular and containerized
  - Analysts provide components specific to their analysis
Opportunistic Resources

- Projects to investigate the use of cloud resources for HEP
- Full ATLAS sites using the Rucio Storage Element and PanDA queue demonstrated on Amazon and Google
- Various payloads including analysis, simulation, athenaMT reconstruction have been demonstrate
- Several setups (Spot and Preemptible instances, virtual machines with different disk configurations) have been evaluated
- Next steps: Demonstrate features and capabilities not available (or limited) on WLCG and University resources. For example, use of ML tools, analytics and other features of GCP for physics analysis.
Machine Learning

- Artificial intelligence and machine learning are used extensively by ATLAS in all areas of event processing and physics analysis
- Prominent USATLAS examples
  - ONNX Runtime integration in athena to enable more applications of machine learning
  - Distributed training enabled the use of GANs to describe the fluctuations in hadronic showers in the calorimeter in Atlfast3
- Many opportunities to profit from advances in artificial intelligence machine learning
  - ML for simulation in detectors beyond calorimeters
  - ML to reduce event generation time
  - ML-based track reconstruction algorithms