Challenges in HEP computing for the next decade

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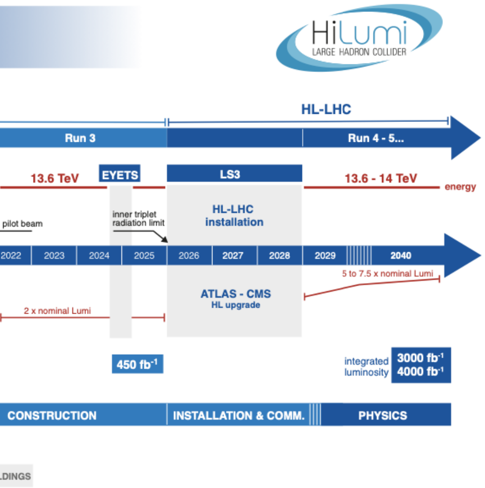
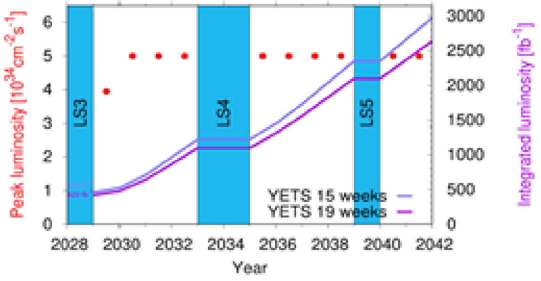
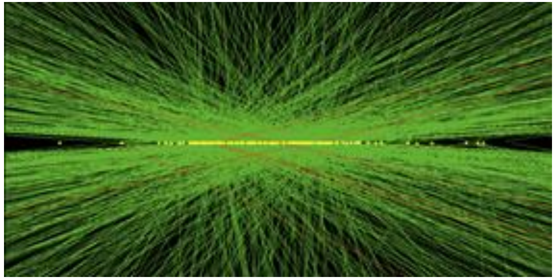
Challenge summary in one paragraph

- The HEP computing challenge is to ensure successful and timely delivery of the best possible physics results from the ongoing and future HEP experiments.
  - **The obvious challenge in the next decade is the HL-LHC upgrade.**

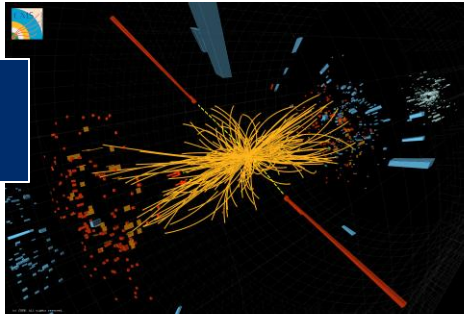




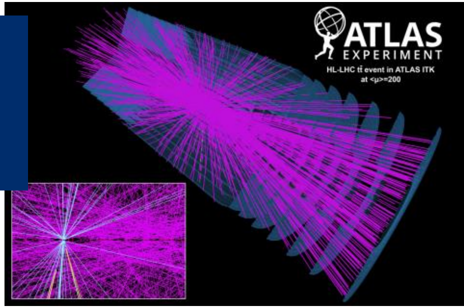
Pile-up collisions, estimated to average 54/140/200 in Run-3/4/5!



2011 Higgs candidate

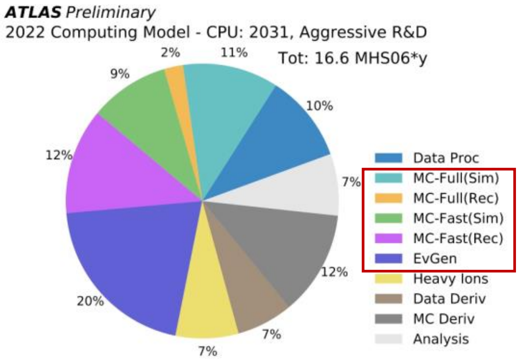


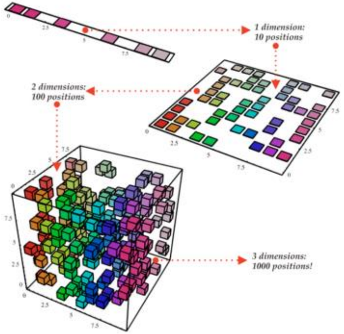
HL-LHC simulated event



Challenge summary in one paragraph

- The HEP computing challenge is to ensure successful and timely delivery of the best possible physics results from the ongoing and future HEP experiments.
  - **In addition to event complexity, the need for an increased volume of simulated Monte Carlo events for precision analysis should not be overlooked!**
    - Machine learning does not negate the need for MC: curse of dimensionality!
      - High-dimensional datasets are at risk of being very sparse: **If you have many free parameters to tune in a DNN, you need a large training volume (and the same for testing and validation)!**





A. Geron: Hands-on ML ..
(book on ML)

In theory, one solution to the curse of dimensionality could be to increase the size of the training set to reach a sufficient density of training instances. Unfortunately, in practice, the number of training instances required to reach a given density grows exponentially with the number of dimensions. With just 100 features (significantly fewer than in the MNIST problem), you would need more training instances than atoms in the observable universe in order for training instances to be within 0.1 of each other on average, assuming they were spread out uniformly across all dimensions.

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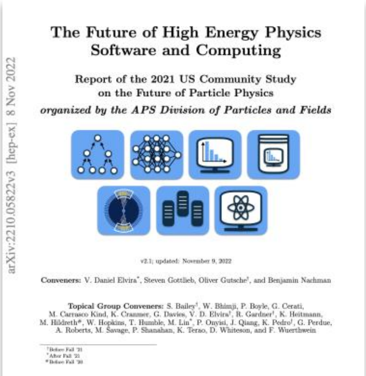
HL-LHC computing planning

- **2017**: HEP Software Foundation Community Whitepaper: a bottom-up exercise. Identify the areas of work to address the HEP challenges of the 2020s.
- **2018**: The first WLCG strategy toward HL-LHC document: a top-down high-level prioritization of the whitepaper, for the LHC needs.
- **2019:** The LHCC review series of HL-LHC computing were initiated , a multistep process tracking the progress towards HL-LHC. As input to the ESPP, WLCG proposed a collaboration model.
- **2020**: review of ATLAS and CMS plans, Data Management (DOMA), offline software, the WLCG collaboration and infrastructure.
- **2021:** update from ATLAS and CMS, common software activities (generators, simulation, foundation software, analysis, DOMA). WLCG presented a joint paper with DUNE and Belle-2 to the Snowmass 2021 process, which detailed the strategic directions needed to address the computing challenges of the experiments over the next decade.
- **2022:** Report from Computational Frontier (CompF) within the Snowmass 2021 process.


ATLAS Software and Computing
HL-LHC Roadmap

HEP computing collaborations for the challenges of the next decade

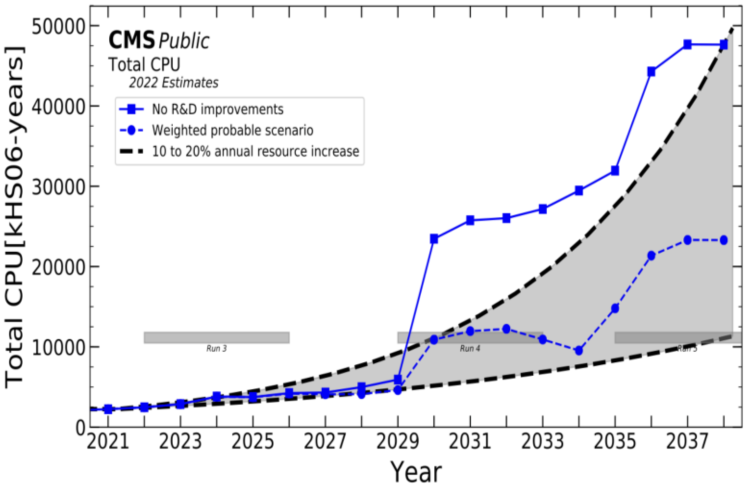

CMS Note
CMS Phase-2 Computing Model: Update Document

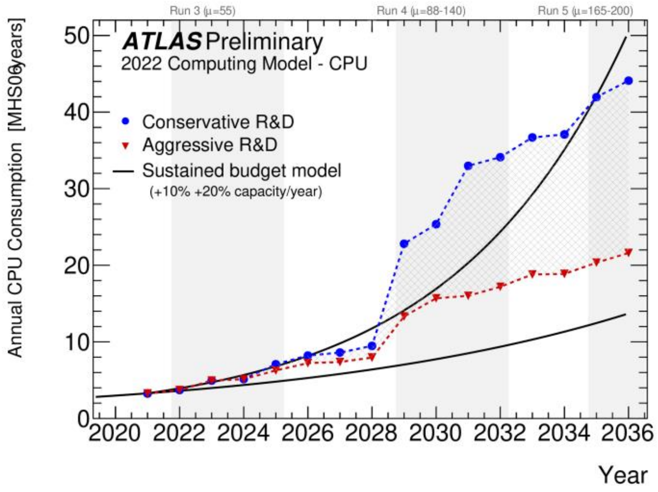


The Future of High Energy Physics Software and Computing
Report of the 2021 US Community Study on the Future of Particle Physics
organized by the APS Division of Particles and Fields
v2.1; updated: November 9, 2022
Conveners: V. Daniel Elvira, Steven Gottlieb, Oliver Gutsche, and Benjamin Nachman

Computing resource projections

- We need to plan well ahead on what we will need, what will be available as resources and what we need to do...





The projected CPU needs of ATLAS and CMS at HL-LHC. Estimates produced for the 2021 HL-LHC computing review and updated in 2022 to reflect the changes in the LHC schedule
ALICE and LHCb will require considerably less in Run-4, while no firm estimates are available for Run-5.

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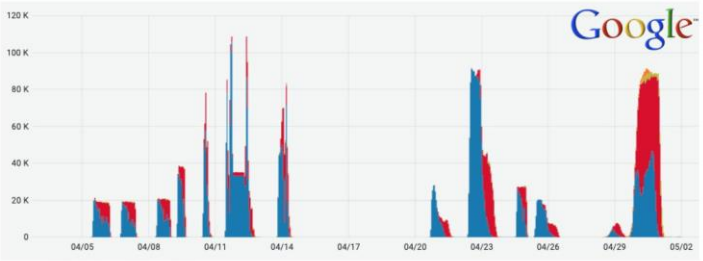
A context: Heterogeneous resources

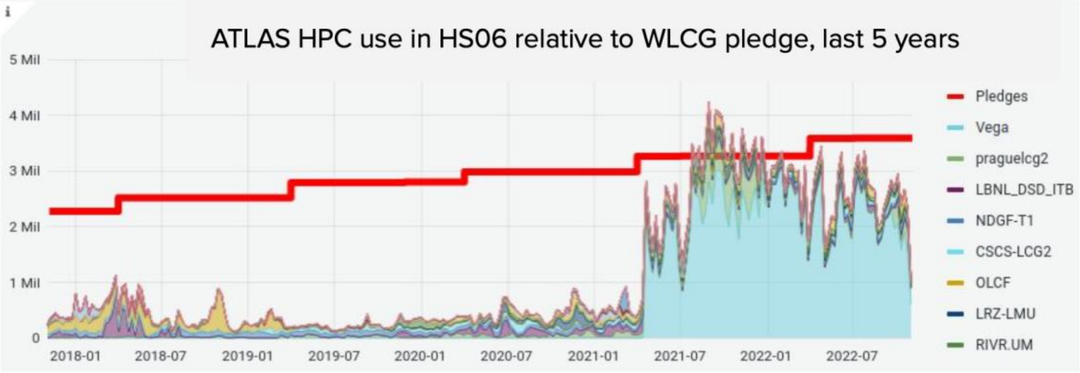
- There are many diverse of computing resources, which we treat as commodities now, but were a challenge to integrate and use (and many lessons to learn from):
  - **Cloud computing:** introduction of containers, specialized data movement...
  - **HPC:** specialized 'edge' services (access, job control), special harware (GPUs), software requirements and data service.
  - **WLCG distributed computing :** a big success story, needing constant vigilance to respond to the evolving computing landscape!
- Integrating all of these takes time! So we need to plan well ahead, invest manpower etc ...

2023 CHEP by D. South

Bursting up to 100k slots for simulation and reconstruction jobs



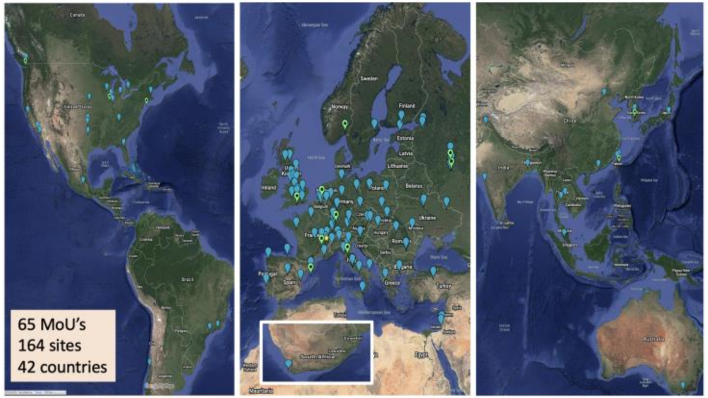
2022 ECFA by D. Britton

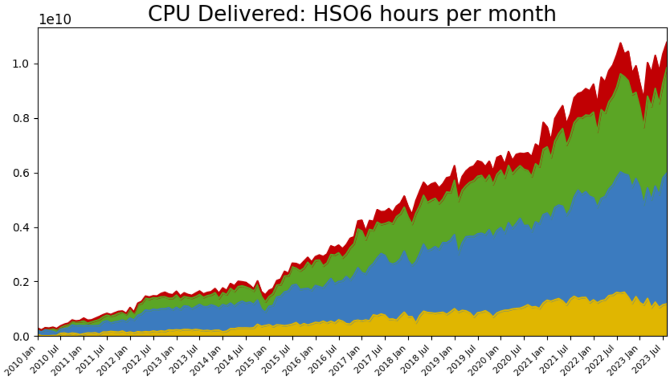


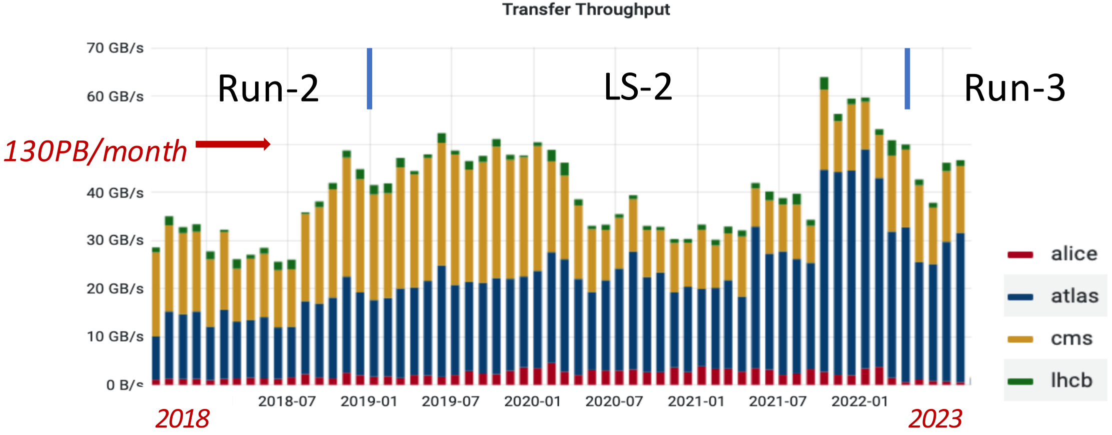
WLCG: distributed computing

WLCG
Worldwide LHC Computing Grid

- **A great success story from HEP,** also a good lesson on finding synergies, establishing common projects across the HEP experiments and scientific community…
  - A system with a lot of components!
  - **Need to sustain this crucial effort!**
  - A model where we diverged from business solutions.







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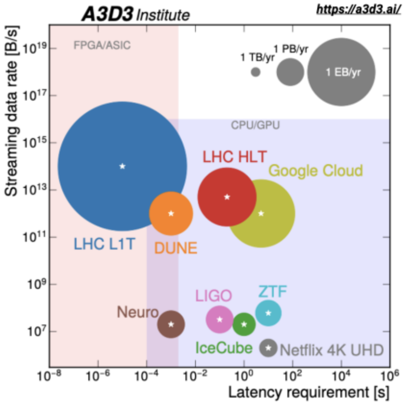
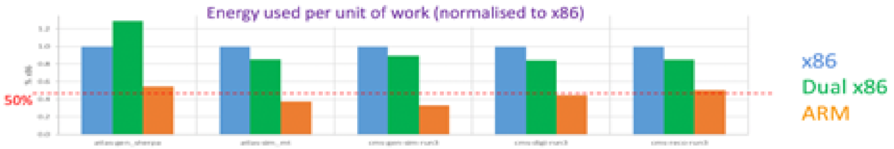
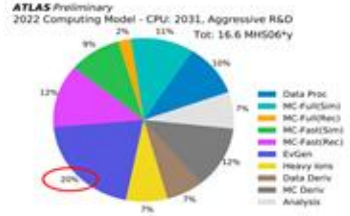
What is out there

- **The HEP paradigm in computing has always been to try out, and use if feasible, everything 'out there' both in terms of hardware and software.**
- **Current challenges being addressed:**
  - **GPUs** (in **HPC**s): massive parallelization, Machine Learning toolkits
  - **ARMs**: energy efficiency,
  - **FPGAs**: speed, ML-readiness,
  - (See Graeme's and Lukas' talks on software and ML !)
- A lot of these are 'self-fullfiling prophecies': we started using HPCs with statistical limit calculations ('MC toys') and MC Generation.
- ... and Quantum Computing is on the horizon!



2022 ECFA by D. Britton





		madevent		
CUDA grid size		8192		
$gg \to t\bar{t}ggg$	MEs precision	$t_{TOT} = t_{Mad} + t_{MEs}$ [sec]	N_{events}/t_{TOT} [events/sec]	N_{events}/t_{MEs} [MEs/sec]
Fortran	double	1228.2 = 5.0 + 1223.2	7.34E1 (=1.0)	7.37E1 (=1.0)
CUDA	double	19.6 = 7.4 + 12.1	4.61E3 (x63)	7.44E3 (x100)
CUDA	float	11.7 = 6.2 + 5.4	7.73E3 (x105)	1.66E4 (x224)
CUDA	mixed	16.5 = 7.0 + 9.6	5.45E3 (x74)	9.43E3 (x128)

NVidia V100, Cuda 11.7, gcc 11.2

Custom or common or … ?

- **We want to use as much commodity software products as possible, to minimize cost and manpower :**
  - In some cases, using commercial libraries, e.g. for state-of-the-art Machine Learning (pyTorch, TensorFlow etc.) is a straightforward choice for using ML tools in HEP (see talk by Lukas).
- **…but there is lot still specific to HEP** (and/or science):
  - specific tools for simulation (Geant4), data persistency and analysis (ROOT),
  - experimental analysis frameworks tying tools together,
  - WLCG with tools for distributed computing and data handling,
- ***and these all need long-term continuity of support !***
  - To share the load and optimize resources, a lot of effort has been made (e.g. HSF) (see talk by Graeme)

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Towards commonality beyond HEP

- **EOSC - European Open Science Cloud**
  - A cloud for research data in Europe allowing seamless access to data and interoperable services.
  - Federate existing infrastructures, National data centres and research infrastructures, allowing researchers and citizens to publish, access, re-use data.
- **ESCAPE - European Science Cluster of Astronomy & Particle Physics** Research infrastructures (ESFRI projects: particle and nuclear physics, gravitational waves, etc.)
  - Develop common infrastructure solutions for particle physics and astronomy facilities
  - Push the state-of-the-art in data mgmt. and computing R&D
  - Address common challenges for data preservation,
  - sustainability, open access...

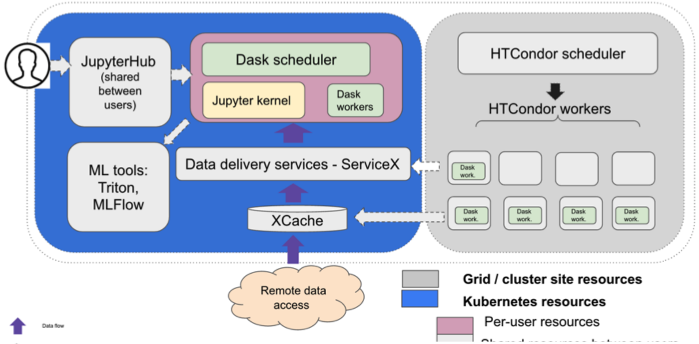
https://projectescape.eu

https://eosc-portal.eu

Change in usage paradigms

- What should also not be neglected are the ways 'users' want to use the computing resources and software environment:
  - Today **jupyter notebooks/browser frontend** is the desired/expected approach.
  - Served by **Analysis Facilities,** envisaged by the HL-LHC computing model upgrades.

CHEP 2023 talk by Elena Gazzarrini, Oksana Shadura, Alexander Held



jupyter – interface to run preliminary analysis

docker, GitLab, GitHub – containerised environments on public repositories

CERN Virtual Machine FS (CVMFS) installed

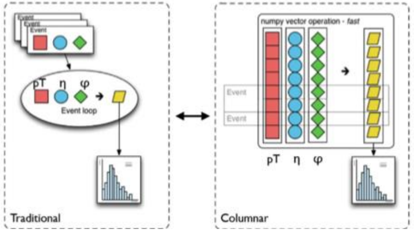
zenodo – client libraries and software installed to interact with underlying services

ceph – CephFS volumes provided as shared, temporary storage solution

IRIS-HEP Strategic Plan for the Next Phase of Software Upgrades for HL-LHC Physics

February 3, 2023 - Version 1.0

https://arxiv.org/abs/2302.01317



Coffea Analysis Framework

ROOT Data Analysis Framework

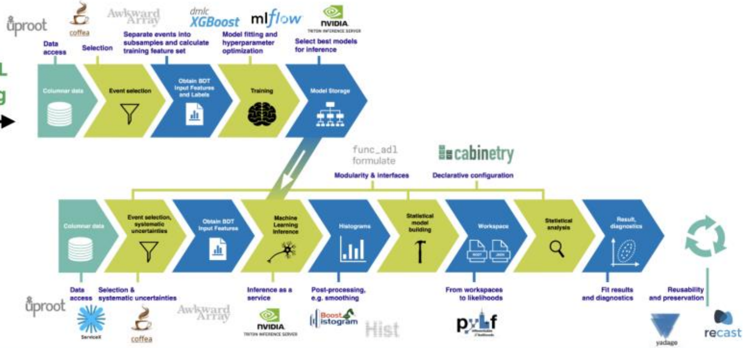
ROOT RDataFrame

DASK

Apache Spark

Parsl

new: ML training



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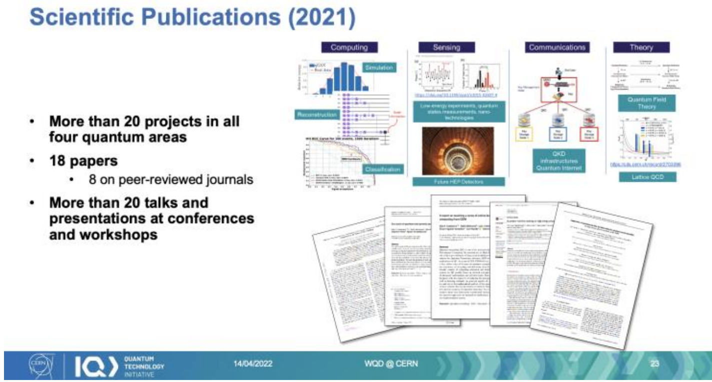
Quantum Computing

2022 JENAS Seminar

- **We need to find out, what we can use it for in HEP successfully.**
  - **Without active participation in existing efforts (e.g. EuroHPC), we might not provide sufficient feedback and encouragement.**
    - Start with MC generators, statistical analysis, (ML) data analysis …
  - We could assume that that successful fault tolerance is achieved in the next decade.
    - We need to learn how to write algorithms, use existing tools for validation, how to integrate these resources.
    - Build partnerships, HEP, wider science community and industry.
  - Quantum Computing expertise also in high demand, can attract manpower!
  - (see the talk by Donatella for details!)



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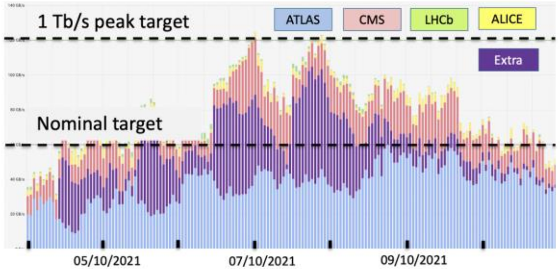
Networks!

- **Often considered a commodity, but a very precious resource!**
- Networks are the backbone of WLCG, which supports the core functions of data acquisition archival and processing!
- Networks also need to be interfaced with HPC centers and Cloud providers.
- IPv4 will need to remain supported at least a few more years for legacy workflows that cannot handle IPv6.
  - IPv6 networks allow new features to be taken advantage of, like Software Defined Networks
- A series of four data/network challenges before HL-LHC to demonstrate full capability
  - The first “10%” challenge took place in October 2021, in preparation for Run-3. The 2nd challenge (Feb. 2024) will be to at least double this. Preparation workshop in Nov. 2023
  - Challenges are end-to-end tests including storage, protocols, networks, and data management services (e.g. Rucio, FTS,...)



Run-3 targets met:

- Nominal transfer rate sustained
- Peak transfer rate reached

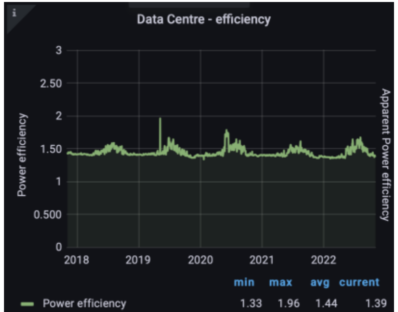
GÉANT Global Connectivity

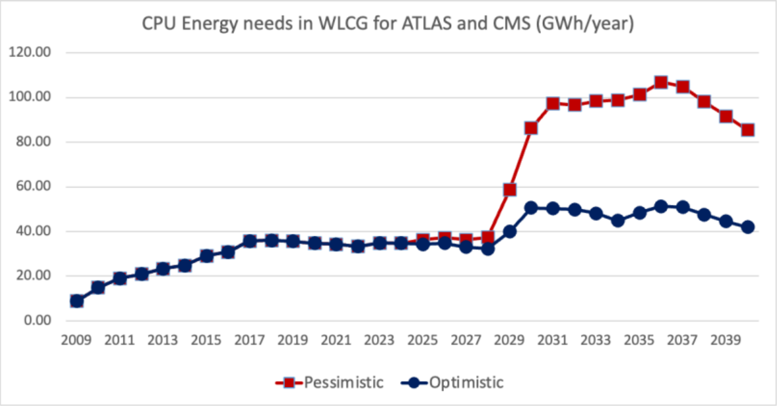
ESnet

Energy efficiency

- The electricity costs have been an unexpected development in the last couple of years.
- **Environmental impact needs proper addressing!**
- **What to do:**
  - Using GPU and ARM architectures could help, but porting of software non-trivial (more in Graeme's talk).
  - Efficient **cooling** of facilities is also important.
  - **There is no magic wand, however.**

The peak of energy need happens in 2036 (start of Run-5): 400% higher than 2022 in the pessimistic scenario and 50% higher in the optimistic scenario.

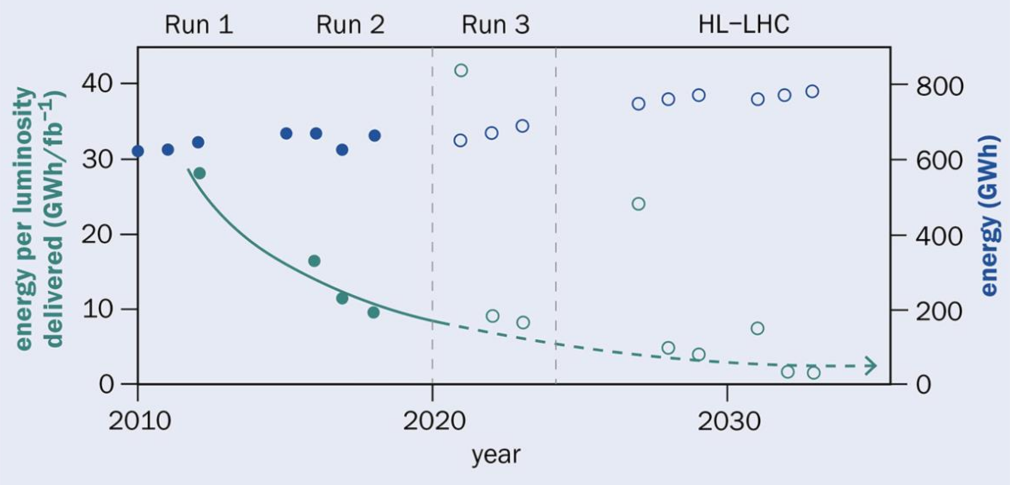




New Key Performance Indicator for HEP facilities

- The GWh/fb–1 metric has now been adopted by CERN as a key performance indicator (KPI) for the LHC (article in CERN Courier)
- **It represents the amount energy needed to produce a given amount of data.**

Inclusive, from accelerator to data analysis...



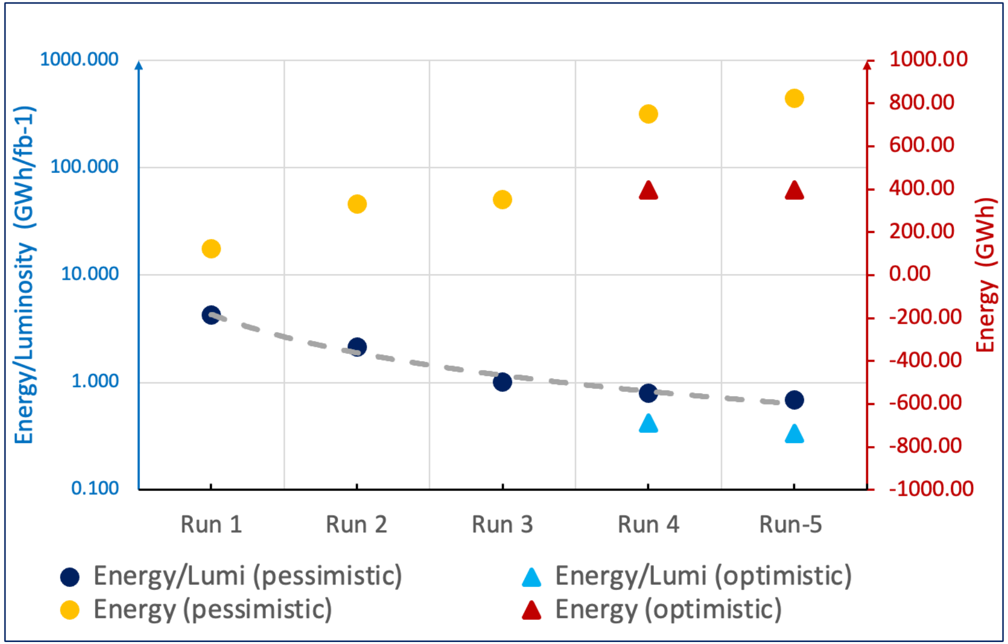
Greener physics Energy consumed (blue) and per luminosity delivered (green) by previous (solid circles) and future (open circles) LHC runs. Credit: S Claudet

New Key Performance Indicator for WLCG

In WLCG GWh/fb^{-1} represent the energy needed **to analyse the data!**

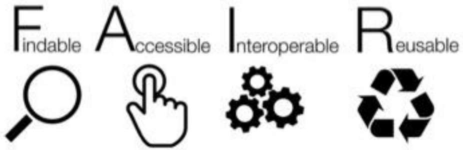
The scale on the right **(RED)** shows the energy and the scale on the left **(BLUE)** shows GWh/fb^{-1} (log!)

Energy needs in Run-4 and Run-5: +100% compared to Run-2 in the **pessimistic** scenario, only +10% in the **optimistic** scenario



GWh/fb^{-1} decreases by a factor 10 between Run-1 and Run-5 (exponential trend fits well)
In Run-5, GWh/fb^{-1} in the **optimistic** scenario is half compared to the **pessimistic** scenario

Addressing the FAIR approach



- **Targeting the open sharing of scientific knowledge and the re-use of research outputs!**
  - Work is ongoing in adopting FAIR principles to the whole lifecycle of data products, algorithms and software..
  - **It does require additional manpower and commitment!**
- To list some key aspects:
  - Development of authentication and authorisation standards
  - Open access and data sharing across communities (from data lakes to Zenodo)
  - Also requires workflows to be sharable - cf. Virtual Research Environments and the tools in Dark Matter and Gravitational Waves communities.
- **To make FAIR a success it has to be possible, easy, normal practice, rewarded and, eventually, required!**
  - **This is a significant technical and cultural challenge - it's certainly not 'free' ...**
  - CERN and most of HEP institutes involved!

Security!

- **An often overlooked aspect:** Our data, identities and computing resources can be corrupted/expoited by malicious agents.
- **In fact a lot of effort continuously invested ‘behind the scenes’**
- **For distributed computing, the access/security is especially complex**: a system of certification authorities with X509 certificates and certificate proxies was established about two decades ago
  - In the last few years, WLCG has started transitioning from X509 user certificates and VOMS proxies towards using WLCG **tokens** instead **- a big change!**
  - Tokens are a modern standard, so introducing them will make our stack more capable to integrate modern technologies.
    - However, being more standard means more attackers know how to exploit them …
    - Rates, lifetimes, scopes, (strict) policies…
  - A timeline with tentative milestones was published in August 2022
  - Computing – in production for OSG & WLCG, WIP for EGI Check-in tokens.
  - Data – discussions ongoing between stakeholders:
    - Experiments, CTA, dCache, DIRAC, Echo, EOS, FTS, IAM, Rucio, StoRM, XRootD, …
  - **Tentative goal (~2026): users no longer need X509 certificates!**

Summary

- **Computing in HEP is a dynamic and challenging activity, always with the need to evolve …**
  - Hardware and software evolution calls for a periodic redesign of the computing models and tools in HEP:
    - **Ongoing challenge with heterogeneous resources (**HPC, Cloud, ARM, …): re-design and re-write of a lot of components, from job and data management tools to experiment software frameworks, event generation, detector simulation, reconstruction algorithms etc… (Graeme will say more about this).
    - **Re-design computing and software infrastructure for AI/ML as well as end-user analysis**, with a special emphasis on new approaches (Lukas will give a detailed insight into this).
    - **In addition, plan for future hardware developments** like QC (Donatella will give a detailed insight into this). It takes time to deliver production level software and operational models, and the process is demanding in person power with rare skills (in science and business!).
  - We need collaboration with other projects and sciences with similar computing challenges and focus on scale, functionality, sustainability, and efficiency of future HEP computing.