Software e computing in LHCb: la sfida di Run3 (e oltre)

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Outline



The LHCb experiment

- LHCb was designed to study CPviolation and search for New Physics phenomena in heavy flavour (beauty and charm) quark sector
- Single-arm spectrometer, fully instrumented in pseudo rapidity range $2 < \eta < 5$
 - solid angle coverage ~ 4%, 40% B hadrons
- Thanks to its excellent performance, the LHCb detector also gave crucial insights and world-class measurements in other sectors e.g.
 - CP violation in charm
 - Hadron spectroscopy (tetraquarks, pentaquarks...)
 - Electroweak physics
 - Cross-section measurements in fixedtarget mode
 - Heavy-ion physics





The LHCb experiment

- Many of LHCb results obtained in Run1 and Run2 are dominated by statistical uncertainties
- An upgrade of LHCb has therefore been planned and it is currently underway to take data in Run3 and beyond





The LHCb upgrade in a nutshell

- An LHCb Upgraded detector is being installed in 2019-2021 (LHC LS2) and it will take data in Run 3 (2022-2024) and beyond.
- The motivation is to boost the physics output by taking advantage of the huge rate of heavy-flavour production at the LHC. This will be achieved by
 - Raising the instantaneous luminosity by a factor five to 2 x 10³³cm⁻²s⁻¹
 - Number of visible interactions x5 larger
 - Implementing a full software trigger
 - to overcome the limitations of L0 hardware trigger
- Huge increase in precision, in many cases to the theoretical limit, and the ability to perform studies beyond the reach of the current detector.
- Flexible trigger and unique acceptance also opens up opportunities in other topics apart from flavour ('a general purpose detector in the forward region')
- Necessary to redesign several sub-detectors and their readout

CERN-LHCC-2012-007

The upgraded LHCb detector for Run 3



Chris Burr • LHCb full-detector real-time alignment and calibration: Latest developments and perspective • CHEP 2018, Sofia CNAF Seminar, Feb 23rd 2021 C. Bozzi, LHCb Software and Computing

CERN-LHCC-2012-007

The upgraded LHCb detector for Run 3



A big challenge in data handling

- Major expansion of LHCb physics programme through:
 - 5-fold increase in instantaneous luminosity
 - 4x10³² to 2x10³³ cm⁻²s⁻¹
 - Full software trigger at 30MHz inelastic collision rate
 - Factor 2 increase in trigger selection efficiency
- Order of magnitude increase in physics event rate to storage
- Pile-up increase
 - Factor 3 increase in average event size
- 30x increase in throughput from the upgraded detector
 - Without corresponding jump in offline computing resources

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Into Computing Resources

O RLY[?]

Harry Houdini

Outline



Run1 + Run2 trigger



Hardware trigger: based on muon detectors and calorimeters
 Run 2

- Data buffered in between two software trigger stages
- Allows for real-time alignment and calibration Offline-quality reconstruction within the trigger

Luminosity increase: x5

- More interaction vertices per collision of proton bunches, more tracks, more signal
- Beauty and charm signal rates: 1-10MHz
- Almost all events will have a b or c hadron

in Run 3





The MHz signal era

| | Signal/ | Turning | kinomotion | Tuisson stustom | Triggor | 10° | Ē | |
|-------|--------------|---------|------------|--------------------|------------------|-------------------------|--|-------------------|
| | background | signal | kinematics | mgger strategy | efficiency | 10 ⁷ | Ē | |
| | 0 | rates | | | | 10 ⁶ | (mb) | |
| GPD | Rare events, | <100kHz | High pT | Local signatures, | Cut at high pT | 10 ⁵ | | |
| ATLAS | background | | | Reject | Work at | 10" | | |
| ′CMS) | dominated | | | background | efficiency | 10° | Ξ (μb) [σ _{jet} (Ε _τ ^{jet} > | 1 |
| | | | | select rare | plateau | (qu 10' | - | |
| LICh | Lligh crocc | | Low nT | No "cimplo" | Cut at low pT | 10 L | (nb) | |
| | sections. | | Low pi | local criteria | Work at | 10 ⁻¹ | ε ο _{jet} (Ε _τ > 10 | 00 |
| | signal | | | Classify decays | efficiency onset | 10 ⁻² | - | |
| | dominated | | | Access as much | edge | 10 ⁻³ | - - (pb) | |
| | | | | information | | 10 ⁻⁴ | | |
| | | | | collision as early | | 10 ⁻⁵ | _ M _H =125 GeV | $\left\{ \right.$ |
| | | | | as possible | | 10 ⁻⁶ | - (fb) | |
| | | | | Read full | | 10 ⁻⁷ | WJS2012 | |
| | | | | detector | | | 0.1 | |



Bottom line: hardware trigger possible at GPDs, not an option for LHCb

The MHz signal era



"From a needle in a haystack to an haystack of needles"

Run 3 trigger



- Remove Hardware trigger in favour of a fully software based one.
- Event reconstruction at collision rate
- Full detector read-out at 40 MHz (visible collision rate: 30MHz)

Run 3 conditions





- Key ingredients for efficient triggering and signal discrimination
 - Primary vertex finding, tracks reconstruction and optimal µ-Identification,
 - Inclusive triggers on signatures with 1&2 "displaced" tracks.
 - Challenge in Run3 is not only to have an efficient trigger, but also be able to identify the topology of events as early as possible in the triggering process: more information than single sub-detector read-out needed
 - Track reconstruction at collision rate required: huge computing challenge

The HLT1 reconstruction sequence



Software performance: early nightmares

- LHCb upgrade online TDR advocates for a trigger farm consisting of O(1000) nodes
- Running HLT1 at 30MHz means that a single node must process O(30k) events/second



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 - take upgrade MC simulation and run HLT1 on it by using the most powerful farm node (at that time: dual-Xenon E5-2630V4, 2*10 cores)
 - Resulting throughput: 6k evts/ s
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 - Resulting throughput: 6k evts/ s
 - 888
- Not unexpected though...

Trigger decisions vs. power of trigger farm



Software performance: somewhat expected

- Run1/2 trigger code single-threaded and scalar
- Evolution trend of faster single- threaded CPU performance broken several years ago.
 - Increase of CPU cores and more execution units.
- Gaudi core framework had been in production without major modifications for 17 years
- Its sequential event data processing model leads to
 - Weak scalability in RAM usage
 - Inefficient disk/network I/O

Trigger decisions vs. power of trigger farm



Software performance: much to gain!

- Modernize Gaudi and make it fit for current and forthcoming challenges
- Several improvements:
 - Better utilization of current multiprocessor CPU architectures
 - Enable code vectorization
 - Modernize data structures
 - Reduce memory usage
 - Optimize cache performance
 - Remove dead code
 - Replace outdated technologies
 - Enable algorithmic optimization





HLT1 on CPUs: mission accomplished

- HLT1 throughput on CPUs has been improved by nearly a factor 5 with no loss on physics performance, surpassing the initial requirement
- This has been made possible by:
 - Rewriting algorithms whose performance used not to be critical (e.g. decodings)
 - Improved use of architecture and intrinsic parallelism, through data model, coding and algorithm design (e.g. velo tracking)
 - Previous experience on operating the current detector, leading to trade-offs and revisited models (e.g. simplified Kalman fit, forward tracking)
- And for most algorithms, all of the above \rightarrow no "one fits all" procedure



Velo trackin Forwar

VeloU

Muor

Other

PV finding Track fit (simpl.) 19.04 %

16.23 %

7.23 %

5.00 %

1.02 9

LHCb Simulation

Throughput = 38198.0 Events/s/node

HLT1 on CPUs: mission accomplished

- HLT1 tested on more recent hardware show even better performance
- A full CPU HLT1 would need fewer than 200 EPYC 7502 servers (AMD CPUs)





HLT1 on GPUs ?

- The Allen project began in February 2018 as an R&D project aimed at providing an HLT1 application running on GPUs
- GPUs offer more theoretical FLOPS in a compact package
- Lower cost than CPUs per theoretical FLOPS
- Many HLT1 tasks are inherently parallel





Allen: salient features

- Implement parallelism on GPUs at the block and thread level
- One event per block along with sub-event parallelism

Memory management:

- Memory allocation is done at the start-up of application
- Custom memory manager for GPU memory
- Not dependent on dynamic libraries for memory allocation



Allen performance (early 2020)

- 60 kHz is the miminum requirement for 30 MHz input rate and 500 GPU cards
- Therefore, Allen can handle the full 30 MHz collision rate with < 500 RTX 2080 Ti GPUs from 2018
- Throughput scales well with theoretical TFLOPs, so Allen will speed up as GPUs improve



HLT1 on CPU and GPU: same physics performance



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Keine leichte Entscheidung...





- Both CPU and GPU proposals carried out in the last years
- Extensive studies and developments on both architectures
- Brand new algorithms and ideas on pattern recognition developed on both architectures
- Benefits of running HLT1 on CPUs:
 - 1. Seamless integration with current infrastructure and operations minimal changes required
 - 2. Easy scalability
- Benefits of running HLT1 on GPUs:
 - 1. Reduce network bandwidth between EventBuilder and filter farms
 - 2. Free up filter farm CPUs for HLT2 only

Final decision : use GPUs for HLT1

• All the work and experience gained for HLT1 reconstruction using CPUs crucial to achieve large speed-up also for the HLT2 reconstruction.

Practical implementation





GPU-equipped event builder PC, with traffic of all three readout cards.



3 PCIe40

Allen performance (today)





GPU-equipped event builder PC, with traffic of all three readout cards.

- Recent Allen optimizations, and usage of consumer NVIDIA cards allow us to deploy up to 4x the processing power foreseen just one year ago
- Using the 3090 results in one card per EB node, with about 10% headroom remaining. To be validated.

HLT2 status

- The same guiding principles used for optimizing the HLT1 application on CPU hold for HLT2
- However, in addition to track reconstruction, also calorimeters and RICHs must be included
- "Converters" also needed for now
 - They close the gap between CPU- and analysisfriendly event model
 - Their real need depends on evolution of analysis model
- More importantly, about 1000 trigger selection lines must also run and be optimised
- HLT2 throughput rate = HLT1 output rate
 - E.g. 3k CPU nodes would be currently needed by HLT2 to match 1MHz HLT1 total rate



HLT2 selection framework

- O(1000) selections:
 - A very complex graph → execution must be optimised
- Data flow:
 - Configurable algorithms properties
 - User-defined inputs/outputs
- Control flow:
 - What should be run and when to stop
- For the execution:
 - Data dependency constructed by matching inputs/outputs
 - Basic nodes ordering respecting data constraints



- Basic node:
 - One algorithm node
 - List of data dependencies
- Composite nodes:
 - Logic (AND | OR | NOT)
 - "Execute all children" or "allow shortcircuiting"

Basic

node

Composite

node

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HLT2 selection framework



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Vectorization of particle selection algorithms

- Two- and three-body particle combination algorithms are being optimised for speed
- Encouraging results when using vector registers on SoA inputs
- Registers must be well filled in order to benefit from vectorization



Outline



From online to offline: Persistency model

- In Run2, LHCb explored another "dimension" of data handling
- In a typical HEP experiment, the trigger rate (kHz, MHz) is often quoted, then the bandwidth (MB/s, GB/s) is determined by assuming an average event size
 - RAW banks are typically streamed to offline for event reconstruction
- ...but if the event reconstruction is done online by the HLT, then one can decide whether to send offline the entire event or only part of it
- At a fixed bandwidth = rate * event_size, one can then increase the rate, and therefore the physics sensitivity of the experiment, by saving only the "interesting" part of an event!

• Selective persistency: write out only the "interesting" part of the event.



- Turbo stream:
 - Miminum output: only HLT2 signal candidates

Limitations: cannot refit tracks and PVs offline, rerun flavour tagging etc. Advantage: Event size O(10) smaller than RAW

• Selective persistency: write out only the "interesting" part of the event.



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Optionally: (parts of) pp vertex (e.g. "cone" around candidate for spectroscopy searches)
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- FULL stream: all reconstructed objects in the event
 - Optionally adding selected RAW banks

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Advantage: Event size O(10) smaller than RAW

- FULL stream: all reconstructed objects in the event
 - Optionally adding selected RAW banks
- TurCal stream: HLT2 candidates and RAW banks

• Used for offline calibration and performance measurement CNAF Seminar, Feb 23rd 2021 C. Bozzi, LHCb Software and Computing

Streams and event sizes in Run 2

 Trigger output saved in 3 different streams using different file format

| Stream | Content | File format |
|-------------|------------------------------------|-------------|
| FULL | Full event information | RDST |
| Turbo | Selected event information | MDST |
| Calibration | Full event information + raw banks | RAW or RDST |

Run 2 event sizes

| stream | event size | event rate | rate | throughput | bandwidth | |
|--------|------------|------------|----------|------------|-----------|---|
| | (kB) | (kHz) | fraction | (GB/s) | fraction | |
| FULL | 70 | 7.0 | 65% | 0.49 | 75% | E |
| Turbo | 35 | 3.1 | 29% | 0.11 | 17% | |
| TurCal | 85 | 0.6 | 6% | 0.05 | 8% | |
| total | 61 | 10.8 | 100% | 0.65 | 100% | Ī |

Event size: Turbo/FULL ~0.5

N.B Turbo event size is an average. It ranges from a few kB (minimal persistence) to full event size

Extrapolation of Run2 rates to Run3 conditions

- With the upgrade conditions several factors need to be applied
 - Luminosity 4*10³² cm⁻²s⁻¹ to 2x10³³ cm⁻²s⁻¹
 - HLT efficiency increase because of removal of L0 hardware trigger
 - Raw event size increase due to pileup, according to simulation
- Without any changes the HLT output rate would increase in Run 3 to 17.4 GB/s

| | Run 2 (GB/s) | Lumi | No L0 | Raw size | Run 3 (GB/s) | |
|-------------|-----------------|------|----------|-------------|-----------------|-------------------|
| Full | 0.49 | x5 | x2 | x3 | 14.7 | Event size: |
| Turbo | 0.11 | x5 | x2 | x1 | 1.1 | Turbo/FULL ~0.167 |
| Calibration | 0.05 | x5 | x2 | x3 | 1.6 | |
| Total | 0.66 | | | | 17.4 | |

Evolution of physics programme

- Moving a larger fraction of the physics programme to Turbo decreases the output bandwidth
- Turbo events are considerably smaller (16 % of Full size)
- Some selections need to stay in Full
 - Keep some flexibility, recover from possible errors, develop new analysis ideas



- For the baseline model we assume 60% of the physics selections currently on FULL stream migrating to Turbo
- Massive migration, not trivial!
- Baseline model assumes 73% of the physics selections on Turbo
- Corresponds to a BW of 10 GB/s

Baseline bandwidth: evolution of the model

- Can we fit 10 GB/s in a reasonable amount of storage resources ?
- First attempt, presented in summer 2018 to LHCC and WLCG resulted in an amount of disk 3.5 times larger than what expected in a "constant budget" evolution model !
- mitigation strategies clearly needed



First attempt to fit upgrade data on disk (summer 2018)

Baseline bandwidth: evolution of the model

Idea! Use cheap storage as a safety net :

- save the desired BW on tape
- Profit of *sprucing* to reduce data volume to disk.
- ...but with the possibility of reprocessing
- Operationally more challenging
- Much safer from the physics point of view



- Similar to Turbo trigger selections
- High event retention (~80%)
- Use selective persistence to substantially reduce data volume
- Output format is MDST







Data Processing Workflow per Data Taking Year



Bandwidth to and from tape

- CERN and Tier1 tape must keep up with the data throughput coming from online
- During (Extended-)Year-End-Technical-Stops, data will be recalled from tape
- Not a full re-reconstruction, only another filtering & slimming pass
- The staging throughput depends on the time required to fully stage
 - And on the dataset luminosity
- Expect ~4x increase with respect to Run2

| Country | Country Site | | Tape Write BW (GB/s) | |
|-------------|--------------|------|-------------------------|--|
| CERN | | 4.24 | 5.50 | |
| | Tier1 si | ites | | |
| France | CC-IN2P3 | 0.49 | 0.63 | |
| Germany | GridKA | 0.86 | 1.12 1.12 0.44 | |
| Italy | CNAF | 0.86 | | |
| Netherlands | SARA/NIKHEF | 0.34 | | |
| Russia | RRCKI | 0.34 | 0.44 | |
| Spain | PIC | 0.23 | 0.29 | |
| UK RAL | | 1.13 | 1.46 | |
| TOTAL Tier1 | sites | 4.24 | 5.50 | |

What about CPU ?

- CPU is dominated by MC production (~90% of CPU power)
- Expected to be the same at the Upgrade
- Scale current MC production to estimate the CPU needs
- Number of needed MC events scale with luminosity
- Seen "experimentally" in Run 2
- Well justified by physics
 - Events signal-dominated
 - Generally pure selections
 - $L_{int} \ x \ \epsilon_{trig}$ is a good proxy for yield
- Assume the same scaling for Upgrade



Fast(er) simulation

- Assumptions on simulated event volume
 - N. of MC events scales with Lint
 - MC production for a data taking years extends over the following 6 years
 - MC events saved in MDST format (x40 size reduction!)
- Implementation of fast simulation techniques already resulted in a leap in the number of simulated events
 - 2018→2019: 4x and only 30% more CPU



Successful adoption of fast simulations

- Full full Geant4 detector simulation
- PGun single signal particle spawned with kinematics configured to follow distribution (no full pythia event) Factor 50 speed increase
- ReDecay re-use the underlying event but generate and simulate new signal decays every time <u>Eur. Phys. J C78 (2018) 1009</u> Factor 10-20 speed increase
- TrackerOnly simulation Factor 10 speed increase
- SplitSim only simulate full event if required condition is passed e.g. if a photon converts to e+e- Speed up depends on condition



All Events Last 365 Days by Simulation Type

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Outline



Data Analysis

- In Run 1 + 2 analysts create nTuples individually ...does not scale well for Run 3
 - 1000s of faulty jobs can be submitted instantly
 - Time consuming O(weeks) for Run 1 + 2 tuples failed jobs re-submitted manually by user
 - No analysis preservation infrastructure
- In Run 3 submit jobs centrally using DIRAC transformation System (Analysis Productions
 - MC data is already produced this way
 - Does not require analyst to babysit jobs
 - Jobs can be tested automatically with GitLab CI
 - Job details/configuration/logs automaticall preserved in LHCb bookkeeping/EOS
 - Automated error interpretation/advice
 - Results displayed on webpage



Offline analysis tools



- Tuples produced using TupleTools creation and saving of variable branches for typical use cases eg. TupleToolTrackInfo
 - Very easy to implement but adds lots of redundant branches can easily save 500+ variables
 - 500GB 10TB of data for a single Run 1+2 analysis nTuples tend to be only used for one analysis
 - **Redesign** of tools such that this redundancy is minimised
- LHCb collaboration uses a wide range of tools C++ /Python/ ROOT/ uproot/ numpy/ pandas/..
- Custom user environments (for use on distributed computing) limited by CVMFS distributions
 - Experimenting with providing analysts the ability to install Conda environments on CVMFS
 - Singularity containers (CERNVM) are used for running legacy applications on grid - looking to expand

Distributed computing

- DIRAC is and remains the LHCb standard for workload and data management
- Current DIRAC design is expected to scale with Run3 workloads and data volumes
- Recent deployments to exploit manycore architectures
 - Use case: Marconi-A2 partition at CINECA, 68x4HT = 272 logical processors
 - DIRAC is able to "partition" the node for optimal memory and throughput
 - Using DIRAC "pool", an <u>inner computing</u> <u>element</u>
 - Parallel jobs matching



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Data management

- Keep it simple
 - Reasonably small number of sites with storage
 - CERN + 7 Tier1 + ~15 Tier2 with disk
- Job matching based on where data is located, no remote access (except in case of failure), high efficiency
- No caches, no underlying data movements
- Static number of replicas
- Data popularity studies give reasonable utilization
- Following WLCG standards and their evolution for transfers:
 - FTS, TPC, ...
- Not directly involved, but following DOMA activities





Run 3 Computing Model

- Concepts developed and implemented during Run 2 to become predominant
 - Split HLT → real-time alignment and calibration
 - TURBO stream for majority of physics program → RAW events discarded
 - FULL and CALIBRATION streams to insure flexibility
 → filter & slim offline
- Offline CPU computing needs dominated by simulation
 - Number of events to be simulated scales with luminosity
 - Simulation time per event scales with pileup
 - →CPU simulation explodes → need for faster simulations
- Offline storage driven by trigger output bandwidth
 - MC saved in μDST , so little impact on storage



Storage requirements - disk



- Pledge evolution assumes a "constant budget" model (+20% more every year)
- Given as a gauging term

- Max deviation from this model: x1.6
- In line with the model by the end of LS3

Storage requirements - tape



| LH | Cb | 2020 | 2021 | 2022 | 2023 | 2024 | 2025 | 2026 | Average |
|------|----------|------|------|------|------|------|------|------|---------|
| ТАРГ | PB | 92 | 120 | 220 | 320 | 420 | 420 | 420 | |
| TAPE | Increase | | 30% | 84% | 45% | 31% | 0% | 0% | 29% |

- Pledge evolution assumes a "constant budget" model (+20% more every year)
- Given as a gauging term

- Max deviation from this model: x1.8
- \sim in line with the model by the end of LS3
- N.B. tape is considered "cheap"

CPU requirements



| LH | Cb | 2020 | 2021 | 2022 | 2023 | 2024 | 2025 | 2026 | Average |
|-----|----------|------|------|------|------|------|------|------|---------|
| CDU | kHS06 | 607 | 1170 | 1256 | 2256 | 3256 | 4256 | 5256 | |
| CPU | Increase | | 93% | 7% | 80% | 44% | 31% | 23% | 35% |

- Pledge evolution assumes a "constant budget" model (+20% more every year)
- Given as a gauging term

- Max deviation from this model: x1.8
- Plan to use opportunistic resources, which are however not granted
- Online farm can be used opportunistically when idle (as we do now)

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Outline



Towards a phase-II upgrade?

- The recent European Strategy on Particle Physics calls for full exploitation of the high-luminosity LHC
 - Unique opportunity to reach the ultimate precision in flavour physics observables
- R&D in the past couple of years towards a phase-II upgrade of LHCb with yet another factor 5 increase in luminosity (→10³⁴ cm⁻² s⁻¹)
- Technologically challenging for detector technologies...
 - increased pileup, occupancies, radiation
 - Timing information (~10ps) needed to isolate signals



CERN-LHCC-2017-003 CERN-LHCC-2018-027



Physics Case for an LHCb Upgrade II



Opportunities in flavour physics, and beyond, in the HL-LHC era

Towards a phase-II upgrade?

- ...and software & computing
 - Aggressive data reduction by moving processing even closer to the real detector: e.g. real-time tracking with FPGAs
 - A simple extrapolation of Run3 computing model does not scale: resource requirements explode, R&D is needed to exploit new dimensions of computing

