Meeting Future Software Challenges in High-Energy Physics

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HL-LHC and the Intensity Frontier

Our mission:

- Exploit the Higgs for SM and BSM physics
- b, c, tau physics to study BSM and matter/anti-matter
- Dark matter
- QGP in heavy ion collisions
- Neutrino oscillations and mass
- Explore the unknown
An Overview of HEP Software

- >50 millions of lines of code, mainly C++, a lot of Python
  - Commercial development cost ~500M CHF
- Critical part of our physics production pipeline, from triggering all the way to analysis and final plots as well as simulation
- Significant pieces of software are already shared by most experiments:
  - Event generators, Geant4, ROOT

This is the “traditional” view and how this changes in the future is an important topic for our discussions.
HEP Computing

- Tasks broken into jobs by experiment production systems (levels of parallelism)
  - Tasks $\rightarrow$ job $\rightarrow$ events $\rightarrow$ algorithms
- LHC experiments use
  - 1M CPU cores every hour of every day
  - Store 1000PB of data (600/400PB tape/disk split)
  - We are in the exabyte era already
  - 100PB of data transfers per year (10-100Gb links)
- This is a huge and ongoing cost in hardware and human effort
- With significant challenges ahead of us to support our ongoing physics programme
Technology Evolution

- Moore’s Law continues to deliver increases in transistor density
  - But, doubling time is lengthening
- Clock speed scaling failed around 2006
  - No longer possible to ramp the clock speed as process size shrinks
  - Leak currents become important source of power consumption
- So we are basically stuck at ~3GHz clocks from the underlying $Wm^{-2}$ limit
  - This is the *Power Wall*
  - Limits the capabilities of serial processing
- Memory access times are now ~100s of clock cycles
  - Poor data layouts are catastrophic for software performance
Decreasing Returns over Time

- Conclusion is that diversity of new architectures will only grow
- Best known example is of GPUs

[link]
Drivers of Technology Evolution

- **Low power devices**
  - Driven by mobile technology and Internet of Things

- **Data centre processing**
  - Extremely large clusters running fairly specialist applications

- **Machine learning**
  - New silicon devices specialised for training machine learning algorithms, particularly low precision calculations

- **Exascale computing**
  - Not in itself general purpose, but poses many technical problems whose solutions can be general - HEP pushed to use HPC centres, especially in US

- **Energy efficiency is a driver for all of these developments**
  - Specialist processors would be designed for very specific tasks
  - Chips would be unable to power all transistors at once: dark silicon is unlit when not used
Hardware Evolution in a Nutshell

Oh brave new world!
That has such people in it...

c. 2000

CPU
Memory
Spinning Disk
Tape

c. 2019

CPU
L1 Cache
L2 Cache
L3 Cache
Persistent Memory / On-die DRAM
SSD Cache
Spinning Disk
Network (inc. Wide Area)
Tape

Device BUS / Network
Device Memory
GRU / FPGA
Software Challenges and Opportunities
Concurrency

● The one overriding characteristic of modern processor hardware is concurrency
  ○ SIMD - Single Instruction Multiple Data (a.k.a. vectorisation)
    ■ Doing exactly the same operation on multiple data objects
  ○ MIMD - Multiple Instruction Multiple Data (a.k.a. multi-threading or multi-processing)
    ■ Performing different operations on different data objects, but at the same time

● Because of the inherently parallel nature of HEP processing a lot of concurrency can be exploited at rough granularity
  ○ Run many jobs from the same task in parallel
  ○ Run different events from the same job in parallel

● However, the push to highly parallel processing (1000s of GPU cores) requires parallel algorithms
  ○ This often requires completely rethinking problems that had sequential solutions previously, e.g. finding track seeds via cellular automata (TrickTrack library, CMS and FCC)
Heterogeneity

- There are a lot of possible parallel architectures on the market
  - CPUs with multiple cores and wide registers
    - SSE4.2, AVX, AVX2, AVX512, Neon, SVE, Altivec/VMX, VSX
  - GPUs with many cores; FPGAs
    - Nvidia (many generations - often significantly different), AMD, Intel, ...

- In addition there are ‘far out’ architectures proposed, like Intel’s Configurable Spatial Architecture

- Many options for coding, both generic and specific:
  - Cuda, TBB, OpenACC, OpenMP, OpenCL (→ Vulcan), alpaka, Kokkos, ...

- Frustratingly no clear winner, mutually exclusive solutions and many niches
  - One option for now is to isolate the algorithmic code from a ‘wrapper’ that targets a particular device or architecture - approach of ALICE for their GPU/CPU code
  - Hiding details in a lower level library (e.g. VecCore) also helps insulate developers
Data Layout and Throughput

- Original HEP C++ Event Data Models were heavily inspired by the Object Oriented paradigm
  - Deep levels of inheritance
  - Access to data through various indirections
  - Scattered objects in memory
- Lacklustre performance was ~‘hidden by the CPU and we survived LHC start
- In-memory data layout has been improved since then (e.g. ATLAS xAOD)
  - But still hard for the compiler to really figure out what’s going on
  - Function calls non-optimal
  - Extensive use of ‘internal’ EDMs in particular areas, e.g. tracking
- iLCSoft / LCIO also proved that common data models help a lot with common software development
- Want to be flexible re. device transfers and offer different persistency options
  - e.g. ALICE Run3 EDM optimised for message passing and the code generation approaches in FCC-hh PODIO EDM generator
Machine Learning

- Machine learning, or artificial intelligence, used for many years in HEP
  - Algorithms learn by example (training) how to perform tasks instead of being programmed
- Significant advances in the last years in ‘deep learning’
  - Deep means many neural network layers
  - Fast differentiability and use of GPUs
- Rapid development driven by industry
  - Vibrant ecosystem of tools and techniques
  - Highly optimised for modern, specialised hardware

ML minimisation problem - do this minimisation with $10^6$ variables...

An example of a modern ML architecture
Machine Learning in HEP

- Better discrimination
  - Important input for analysis (see improvements with Higgs)
  - Also used at HLT as inference can be fast (N.B. training can be slow!)
  - HEP analogies to image recognition or text processing

- Replace expensive calculations with trained output
  - E.g. calorimeter simulations and other complex physical processes

- There are significant opportunities here
  - Need to combine physics and data science knowledge
  - Field evolves rapidly and we need to deepen our expertise

- Integration into our workflows is not at all settled
  - Resource provision, efficient use, heterogeneity and programming models pose problems
  - Training deep models may require significant resources

Table 1 | Effect of machine learning on the discovery and study of the Higgs boson

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Years of data collection</th>
<th>Sensitivity without machine learning</th>
<th>Sensitivity with machine learning</th>
<th>Ratio of $P$ values</th>
<th>Additional data required</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMS$^{24}$ $H \rightarrow \gamma\gamma$</td>
<td>2011–2012</td>
<td>$2.2\sigma$, $P = 0.014$</td>
<td>$2.7\sigma$, $P = 0.0035$</td>
<td>4.0</td>
<td>51%</td>
</tr>
<tr>
<td>ATLAS$^{43}$ $H \rightarrow \tau^+\tau^-$</td>
<td>2011–2012</td>
<td>$2.5\sigma$, $P = 0.0062$</td>
<td>$3.4\sigma$, $P = 0.00034$</td>
<td>18</td>
<td>85%</td>
</tr>
<tr>
<td>ATLAS$^{99}$ $VH \rightarrow bb$</td>
<td>2011–2012</td>
<td>$1.9\sigma$, $P = 0.029$</td>
<td>$2.5\sigma$, $P = 0.0062$</td>
<td>4.7</td>
<td>73%</td>
</tr>
<tr>
<td>ATLAS$^{41}$ $VH \rightarrow bb$</td>
<td>2015–2016</td>
<td>$2.8\sigma$, $P = 0.0026$</td>
<td>$3.0\sigma$, $P = 0.00135$</td>
<td>1.9</td>
<td>15%</td>
</tr>
<tr>
<td>CMS$^{100}$ $VH \rightarrow bb$</td>
<td>2011–2012</td>
<td>$1.4\sigma$, $P = 0.081$</td>
<td>$2.1\sigma$, $P = 0.018$</td>
<td>4.5</td>
<td>125%</td>
</tr>
</tbody>
</table>

Use of Generative Adversarial Networks to simulate calorimeter showers, trained on G4 events (S. Vallacorsa)

Machine learning at the energy and intensity frontiers of particle physics,

https://doi.org/10.1038/s41586-018-0361-2
HEP Software and Computing and the HSF Initiative
Software at the HL-LHC

- Pile-up of ~200 ⇒ particularly a challenge for charged particle reconstruction
  - Inner trackers and CMS High Granularity Calorimeter
- HEP software typically executes one instruction at a time (per thread)
  - Since ~2013 CPU (core) performance increase is due to more internal parallelism
  - x10 with the same HW only achievable if using the full potential of processors
    - Major SW re-engineering required (but rewriting everything is not an option)
  - Co-processors like GPUs require that this problem is solved
- Increased amount of data requires to revise/evolve our computing and data management approaches
  - We must be able to feed our applications with data efficiently
- **HL-LHC salvation will come from software improvements, not from hardware**
Challenges for the Next Decade

- HL-LHC brings a huge challenge to software and computing
  - Both rate and complexity rise

- Not just a simple extrapolation of Run 2 software and computing
  - Resources needed would hugely exceed those from technology evolution alone

[Caveat Emptor: 2017 Plots - now updated]
HEP Software Foundation (HSF)

- The LHC experiments, Belle II and DUNE face the same challenges
  - HEP software must evolve to meet these challenges
  - Need to exploit all the expertise available, inside and outside our community, for parallelisation
  - New approaches needed to overcome limitations in today’s code
- Cannot afford any more duplicated efforts
  - Each experiment has its own solution for almost everything (framework, reconstruction algorithms, ...)
- HSF started with a number of workshops and working groups on common topics (packaging, licensing)
- The goal of the HSF is to facilitate coordination and common efforts in software and computing across HEP in general
  - Our philosophy is bottom up, a.k.a. do-ocracy
Community White Paper Inception

- We wanted to describe a **global vision for software and computing** for the HL-LHC era and HEP in the 2020s

- Formal [charge from the WLCG](#) in July 2016
  - Anticipate a "software upgrade" in preparation for HL-LHC
  - Identify and prioritize the software research and development investments
    - i. to achieve improvements in software efficiency, scalability and performance and to make use of the advances in CPU, storage and network technologies
    - ii. to enable new approaches to computing and software that could radically extend the physics reach of the detectors
    - iii. to ensure the long term sustainability of the software through the lifetime of the HL-LHC

- Long process of 1 year, with many working groups and 2 major workshops
A Roadmap for HEP Software and Computing R&D for the 2020s

- 70 page document
- 13 sections summarising R&D in a variety of technical areas for HEP Software and Computing
  - Almost all major domains of HEP Software and Computing are covered
- 1 section on Training and Careers
- 310 authors from 124 institutions

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int main {
    cout << "write software" << endl;
    return 0;
}

HSF Working Groups

- The Roadmap established what challenges the community faced
  - But it did not spell out how to face them in detail

- HSF had adopted a model of working groups from its earliest days
  - These were open groups of people in the community, motivated enough to organise around a common topic, usually at their own initiative

- This model seemed a good one for moving forwards on the key topics
  - We were a little more formal this time around
    - Call for nominations from the whole community, then search committee
    - Significant engagement from LHC experiments and beyond, e.g. Belle II

- The HSF’s role is one of an information conduit and meeting point
  - Report on interesting and common work being done
  - Forum for technical comments and discussion
  - Encourage cooperation across experiments and regions
Some important practical matters!
Copyright and Licensing

● Long neglected inside collaborations
  ○ Code was arbitrarily licensed or unlicensed, copyright assigned to random authors and institutes
  ○ Yet this is essential to be able to
    ■ Open source our software properly
    ■ Combine with other open source projects and collaborate

● Copyright
  ○ Advice to keep this as low a number as practicable as copyright holders decide the licence
  ○ LHC experiments: © CERN for the benefit of collaboration X

● License
  ○ Favour liberal licenses for industry collaboration: LGPL, Apache, MIT
  ○ Definitely avoid GPL for libraries you want other people to use
Software Nuts and Bolts

● Software Tools WG
  ○ Active group promoting best practice for correctness and performance
  ○ There has been a revolution in adopting best open source practice in recent years
    ■ git, GitHub, GitLab, CMake, merge requests, code review, ...
  ○ HSF has an active group promoting best practice for correctness and performance
    ■ Profiling, static analysis

● Packaging WG
  ○ We don’t build our experiment software in isolation
  ○ Need a software stack, incorporating many components from the open source world and HEP community
    ■ This touches deeply on license and license combinations
  ○ Preference for tools that are not home grown and have a wider support base
  ○ Spack (LBNL) and Conda actively being prototyped
Event Generators

- Event generators are the start of the simulation chain
  - At the LHC Run1 only leading order generators were used
  - Negligible CPU consumption compared with detector simulation - no pressure to optimise
- However, with LHC upgrades coming higher order generators become much more important
  - These are inherently much more costly to run
  - Problems of negative weights can increase hugely the samples needed for weighted event samples
- In addition, the theory community, who develop these codes usually work in small teams
  - Recognition for technical improvements is limited/missing

Many electroweak measurement errors dominated by theory (red). B. Hinemann
Event Generators - Technical Improvements

- **HSF/LPCC workshop** in November brought theory and experiment together to look at computing challenges of event generation
  - This was the first workshop of its kind

- **Working group tackling technical challenges**
  - Setting a baseline for further comparisons
  - Understanding how to run generators for best efficiency
  - Support for technical improvements (e.g. thread safety)
  - Porting to other architectures
    - Could be very suitable code to do this with (smaller, self contained code bases, numerically intensive)
    - e.g. building on the work done so far in MadGraph with GPUs

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Ref. J. Tanaka [check]
Detector Simulation

- A major consumer of LHC grid resources today
  - Experiments with higher data rates will need to more simulation
- Faster simulation, with no or minimal loss of accuracy, is the goal
  - Range of techniques have been used for a long time (frozen showers, paramtric response)
  - Key point is deciding when it’s good enough for physics
- Machine learning lends itself to problems like this
  - Calorimeter simulations usually targeted
  - Variational Auto Encoders (VAEs) attempt to compress the data down to a ‘latent space’ - can be randomly sampled to generate new events
  - Generative Adverserial Networks (GANs) train two networks, one to generate events, the other to try to classify as real/fake
  - R&D on lifecycle integration into Geant4 is starting...


LHCb ECal simulated with G4, generated with GAN [F. Ratnikov]
Detector Simulation

- Technical improvement programme helps (and helps everyone)
- GeantV R&D modernises code and introduces vectorisation
  - Speed-ups observed
  - Vectorisation introduces small gains
  - Code modernisation seems to help a lot
- Geant4 now have a new R&D working group that will take studies forward
- Some studies of running Geant4 on GPUs have begun
  - US Exascale Computing Project is funding this
  - Motivated by the next generation of US supercomputers that target exaflop
    - 90-95% of FLOP capacity in GPUs
  - However, migration of physics code is an incredibly tricky business
    - This would be a long haul, but a huge achievement for all of HEP
Reconstruction and Software Triggers

- Hardware triggers no longer sufficient for modern experiments
  - More and more initial reconstruction needs to happen in software
- Close to the machine, need to deal with tremendous rates and get sufficient discrimination
  - Pressure to break with legacy code is high
  - Lots of experimentation with rewriting code for GPUs
    - E.g. LHCb’s Allen project (HLT1 on GPU)
  - ALICE have ported a lot of reconstruction to GPUs and also improved the algorithms a lot
  - CMS Patatrack project has improved physics performance as well
    - Revisiting old code helps!
- Lessons learned keep data model simple, bulk data, be asynchronous, minimise data transfers
Reconstruction and Software Triggers

- **Real Time Analysis (HEP Version)**
  - Design a system that can produce analysis useful outputs as part of the trigger decision
    - If this captures the most useful information from the event, can dispense with raw information
      - *This is a way to fit more physics into the budget*
  - LHCb Turbo Stream has been introduced in Run2 and will be dominant in Run3
  - Whole ALICE data reduction scheme is based around keeping ‘useful’ parts of events (no more binary trigger)
    - O2 → Online/Offline Data Reduction Farm
  - ATLAS and CMS have schemes under development for special handling of samples for which full raw data is unaffordable (aka. data scouting)

<table>
<thead>
<tr>
<th>Persistence method</th>
<th>Average event size (kB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbo</td>
<td>7</td>
</tr>
<tr>
<td>Selective persistence</td>
<td>16</td>
</tr>
<tr>
<td>Complete persistence</td>
<td>48</td>
</tr>
<tr>
<td>Raw event</td>
<td>69</td>
</tr>
</tbody>
</table>

LHCb Run2 Turbo took 25% of events for only 10% of bandwidth
Analysis

- Scaling for analysis level data also a huge challenge for all LHC experiments
- Efficient use of analysis data can come with combining many analyses as carriages in a train like model (pioneered by PHENIX and then ALICE)
  - Also goes well with techniques like tape carousels (ATLAS scheme for rotating primary AOD data from tape systems into a disk buffer)
  - Interest in analysis clusters, specialised for analysis operations over the generic grid resources (WLCG/HSF pre-CHEP workshop 2-3 November)
- Reducing volume of data needed helps hugely
  - CMS ~1kB nanoAOD makes a vast difference to analysis efficiency and “papers per petabyte”
  - Smaller EDM is easier to make efficient
  - Requires analyst agreement on corrections, scale factors, etc.
    - However the alternative is perhaps that your analysis never gets done
Analysis

- Improve analysis ergonomics - how the user interacts with the system to express their analysis
  - Streamline common tasks
    - Handle all input datasets; Corrections and systematics
    - Compute per event and accumulate; Statistical interpretations
  - Declarative models, building on ROOT’s RDataFrame
    - Say what, not how and let the backend optimise
    - E.g. split and merge, GPU execution
- Notebook like interfaces gain ground, as do containers - lots of high level Python
- Interest in data science tools and machine learning is significant for this community - inspiring new approaches (e.g. uproot, awkward array, scikit-hep, Coffea)
  - This is an ecosystem into which HEP can contribute

Many analysis frameworks, multiple per experiment, not well generalised

A. Rizzi, NAIL prototype
Frameworks and Integration

- Increasingly heterogeneous world requires advanced software support infrastructure
  - Software frameworks support use of different devices as well as insulate developers from many of the details of concurrency and threading models
    - Adapt to the new heterogeneous landscape
    - Latency hiding is critical to maintaining throughout
  - Framework development has traditionally been quite fragmented, but new experiments should offer a chance to increase convergence
    - Better to start off together than try to re-converge later (iLCSoft, LArSoft examples of success, albeit without concurrency; Gaudi for LHCb, ATLAS)
    - ALFA for ALICE and FAIR experiments
- New HSF working group being established now (draft mandate)
Training and Careers

- Many new skills are needed for today’s software developers and users
- Base has relatively uniform demands
  - Any common components help us
- LHCb StarterKit initiative taken up by several experiments, sharing training material
  - Links to ‘Carpentries’ being remade (US training projects) - up the level!
- New areas of challenge
  - Concurrency, accelerators, data science
  - Need to foster new C++ expertise (unlikely to be replaced soon as our core language, but needs to be modernised)
- Careers area for HEP software experts is an area of great concern
  - Need a functioning career path that retains skills and rewards passing them on
  - Recognition that software is a key part of HEP now
Meeting the HL-LHC Challenge!

- Already since the Roadmap was written, experiments have made great progress in meeting the HL-LHC challenge
  - Bad software, is extremely expensive
  - Good and clever software allows much more physics to fit in the budget
Conclusions

- We have a wide ranging and ambitious physics programme in HEP and in associated disciplines
  - Our experiments are highly data intensive and require high quality software and computing
- The landscape for software is becoming ever more challenging
  - Working together on common problems is not only the best use of our resources, our funding agencies will mandate it
- HSF is now established to help HEP achieve that goal and marshalls effort around the community
  - Roadmap delivered and active working groups in key areas

*HL-LHC is a challenge and also a great opportunity to improve HEP software*
HSF Getting Involved...

- Join the HSF Forum, hsf-forum@gmail.com
  - Few messages a week with updates, jobs, items of interest
  - Owned by the community - please just post items of relevance

- Join a working group, https://hepsoftwarefoundation.org/what_are_WGs.html
  - Follow the group’s meetings and discussions
  - Suggest a meeting topic

- **Annual meetings and Workshops**
  - Establishing a tradition of a joint meeting with WLCG each Year (next short meeting pre-CHEP, November)

- Propose a new activity area
  - The HSF is there to help gather interest

- Data Analysis
- Detector Simulation
- Frameworks
- Physics Generators
- Packaging
- PyHEP - Python in HEP
- Quantum Computing
- Reconstruction and Software Triggers
- Software/Developer Tools
- Training
- Visualization