Advancing Advances in HEP Software and Computing

Graeme Stewart, CERN EP-SFT

Spåtind 2018 - Nordic Conference on Particle Physics, 2018-01-05
Experimental Particle HL-LHC and 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
- Neutrino oscillations and mass
- QGP in heavy ion collisions
- Explore the unknown
HEP Software and Computing

- High Energy Physics has a vast investment in software
  - Estimated to be around 50M lines of C++
  - Which would cost more than 500M$ to develop commercially
- It is a critical part of our physics production pipeline, from triggering all the way to analysis and final plots as well as simulation
- LHC experiments use about 600k CPU cores every hour of every day and have around 400PB of data stored on disk and 600PB on tape
  - We are in the exabyte era already
- This is a huge and ongoing cost in hardware and human effort
- With significant challenges ahead of us to support our ongoing physics programme
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
Technology Evolution

- Moore’s Law continues to deliver increases in transistor density
  - Doubling time is lengthening
  - IBM recently demonstrated 5nm wafer fabrication
- 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
Technology Evolution

- Many/multi core systems are the norm
  - Serial or multi-process processing is under severe memory pressure
- Co-processors now commonplace
  - GPUs, FPGAs - greater throughput, far more challenging programming model
- Wide vector registers
  - Up to 512 bit
- Feeding data from main memory is a serious problem
  - Deeper cache hierarchy
- Storage capacity climbing
  - 100TB disks possible by HL-LHC, but little I/O improvement expected
- Network capacity keeps growing
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

● 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
Software Challenges for HL-LHC

- Pile-up of ~200 ⇒ particularly a challenge for charged particle reconstruction
- With a flat budget, Moore’s lawish improvements are the real maximum we can expect on the HW side
- 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 are of little use until the problem has been 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
How is our code doing? Simulation on 5 years of Intel CPUs

- Fraction of the potential floating point performance we use has been dropping over time
- CPU manufacturers add wider vectors that we do not take advantage of, or deep pipelines where cache misses are very costly
- Confirms what we have long suspected about the growing performance gap on modern architectures
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 already 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-o-cracy
Community White Paper Inception

- From Spring 2016 discussions, idea started to crystallise at the May 2016 HSF Meeting at LAL
  - 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
CWP process

- **Kick-off workshop** 23-26 January 2017, San Diego
- Groups held workshops and meetings in the subsequent months
  - Broadening the range of participation, often with non-HEP experts participated
- **Workshop in Annecy** 26-30 June started to draw the process to a close
  - 13 Working Groups had made good progress on their chapters
- Both workshops involved ~100 people, mainly US and EU
  - Total number of people involved in the writing process was about 250
  - Many others commenting
CWP - Making a roadmap for the future

- Editorial Board was set up, with the aim of encompassing the breadth of our community
  - Wide regional and experimental representation
- First draft released 20 October
- Second draft released 17 November
- These drafts elicited a *substantial response* from the community, leading to many improvements
- Final version of the document published arXiv: 1712.06982 on 20 December
- In addition there are many *individual working group chapters* giving significant detail on their area of expertise

- Predrag Buncic (CERN) - ALICE contact
- Simone Campana (CERN) - ATLAS contact
- Peter Elmer (Princeton)
- John Harvey (CERN)
- Benedikt Hegner (CERN)
- Frank Gaede (DESY) - Linear Collider contact
- Maria Girone (CERN Openlab)
- Roger Jones (Lancaster University) - UK contact
- Michel Jouvin (LAL Orsay)
- Rob Kutschke (FNAL) - FNAL experiments contact
- David Lange (Princeton)
- Dario Menasce (INFN-Milano) - INFN contact
- Mark Neubauer (U.Illinois Urbana-Champaign)
- Eduardo Rodrigues (University of Cincinnati)
- Stefan Roiser (CERN) - LHCb contact
- Liz Sexton-Kennedy (FNAL) - CMS contact
- Mike Sokoloff (University of Cincinnati)
- Graeme Stewart (CERN, HSF)
- Jean-Roch Vlimant (Caltech)
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
- 274 authors from 117 institutions
- Signing policy: sign the document if you agree with the main observations and conclusions
  - hsf-cwp-ghost-writers@googlegroups.com
- We really actively encourage you to do this as your name indicates the breadth of support in the community

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Physics Event Generators

- Physics event generation starts our simulation chain to enable comparisons with detector events
  - At Leading Order the CPU consumption of event generation is modest
  - At Next-to-leading Order CPU consumption can become important
  - To get a proper handle on rare processes at the HL-LHC Next-to-next-to-leading order, NNLO, will be required for more analyses

- Generators are written by the theory community
  - Need expert help and long term associations to achieve code optimisation
  - Even basic multi-thread safety is problematic for many older, but still heavily used, generators
  - Ongoing maintenance of tools like HepMC, LHAPDF, Rivet is required and needs rewarded
  - Projects such as scalable VEGAS-style integrator and reweighting tools are foreseen
Detector Simulation

- **Simulating our detectors consumes huge resources today**
  - Remains a vital area for HL-LHC and intensity frontier experiments in particular

- **Main R&D topics**
  - Improved physics models for higher precision at higher energies (HL-LHC and then FCC)
    - Hadronic physics in LAr TPCs needs to be redeveloped
  - Adapting to new computing architectures
    - Can a vectorised transport engine be demonstrated to work in a realistic prototype? How painful would evolution be?
  - Fast simulation - develop a common toolkit for tuning and validation
    - Can we use Machine Learning profitably here?
  - Geometry modeling
    - Easier modelling of complex detectors, targeting new computing architectures
Software Trigger and Event Reconstruction

- **Move to software triggers is already a key part of the program for LHCb and ALICE already in Run 3**
  - ‘Real time analysis’ increases signal rates and can make computing much more efficient (storage and CPU)

- **Main R&D topics**
  - Controlling charged particle tracking resource consumption and maintaining performance
    - Do current algorithms’ physics output hold up at pile-up of 200 (or 1000)
    - Can tracking maintain low $p_T$ sensitivity within budget?
  - Detector design itself has a big impact (e.g., timing detectors, track triggers)
  - Improved use of new computing architectures
    - Multi-threaded and vectorised CPU code
    - Extending use of GPGPUs and possibly FPGAs
  - Robust validation techniques when information will be discarded
    - Using modern continuous integration, tackling multiple architectures with reasonable turnaround times

See Andy’s talk next
Today we are dominated by many cycles of data reduction

- Aim is to reduce the input to an analysis down to a manageable quantity that can be cycled over quickly on ~laptop scale resources
- Key metric is ‘time to insight’

Main R&D topics

- How to use the latest techniques in data analysis that come from outside HEP?
  - Particularly from the Machine Learning and Data Science domains
  - Need ways to seamlessly interoperate between their data formats and ROOT
    - Python is emerging as the lingua franca here, thus guaranteeing our python/C++ bindings is critical
- New Analysis Facilities
  - Skimming/slimming cycles consume large resources and can be inefficient
  - Can interactive data analysis clusters be set up?
- Data and analysis preservation is important
Data Processing Frameworks

● **Experiment software frameworks provide the scaffolding for algorithmic code**
  ○ Currently there are many implementations of frameworks, with some sharing between experiments
  ○ All of these frameworks are evolving to support concurrency
    ■ Protect physicists from details and dangers of parallelisation

● **Main R&D topics**
  ○ Adaption to new hardware, optimising efficiency and throughput
    ■ We need the best libraries for this and these will change over time
  ○ Incorporation of external (co)processing resources, such as GPGPUs
  ○ Interface with workload management system to deal with the inhomogeneity of processing resources
    ■ From volunteer computing to HPC job slots with 1000s of nodes
  ○ Which components can actually be shared and how is that evolution achieved?
Data Management and Organisation

- **Data storage costs are a major driver for LHC physics today**
  - HL-LHC will bring a step change in the quantity of data being acquired by ATLAS and CMS

- **Main R&D topics**
  - Adapt to new needs driven by changing algorithms and data processing needs, e.g,
    - The need for fast access to training datasets for Machine Learning
    - Supporting high granularity access to event data
      - Needed to effectively exploit backfill or opportunistic resources
    - Rapid high throughput access for a future analysis facility
    - Processing sites with small amounts of cache storage
  - Do this profiting from the advances in industry standards and implementations, such as Apache Spark-like clusters (area of continued rapid evolution)
    - Of course what we do is not exactly like what they do... structured access to complex data
  - Consolidate storage access interfaces and protocols
  - Support efficient hierarchical access to data, from high latency tape and medium latency network
Facilities and distributed computing

- **Storage and computing today are provided overwhelmingly from WLCG resources**
  - Expected to continue for HL-LHC, but to be strongly influenced by developments in commodity infrastructure as a service (IaaS, commercially this is usually Cloud Computing)

- **Main R&D topics**
  - Understand far better the effective costs involved in delivering computing for HEP
    - This needs to be sensitive to regional variations in funding and direct and indirect costs
      - e.g., smaller sites frequently contribute ‘beyond the pledge’, power and human resources
    - Full model is unfeasible, but providing a reasonable gradient analysis for future investment should be possible
      - Should we invest in better network connectivity or in more storage?
      - Does a data lake make sense for us? Concentrated storage at fewer sites.
  - How to take better advantage of new network and storage technologies
    (software defined networks, object stores or content addressable networks)
  - Strengthen links to other big data sciences (SKA) and computing science; how to share network resources
Machine learning

• Neural networks and Boosted Decision Trees have been used in HEP for a long time
  ○ e.g., particle identification algorithms

• More recently the field has been significantly enhanced by new techniques (Deep Neural Networks) and enhanced training methods
  ○ Very good at dealing with noisy data and huge parameter spaces
  ○ A lot of interest from our community in these new techniques, in multiple fields

• Main R&D topics
  ○ Speeding up computationally intensive pieces of our workflows (fast simulation, tracking)
  ○ Enhancing physics reach by classifying better than our current techniques
  ○ Improving data compression by learning and retaining only salient features
  ○ Anomaly detection for detector and computing operations

• Significant efforts will be required to make effective use of these techniques
  ○ Good links with the broader Machine Learning and Data Science communities required

See Kyle’s talk Thursday
Data, software and analysis preservation

- We seem to be doing well compared to other fields
- Challenge is both to physically preserve bits and to preserve knowledge
  - DPHEP has looked into both
- Knowledge preservation is very challenging
  - Experiment production workflows vary in significant details
  - Variety of different steps are undertaken at the analysis stage, even within experiments
- Need a workflow that can capture this complexity
  - Technology developments that can help are, e.g., containers
- CERN Analysis Preservation Portal forms a good basis for further work
  - Needs to have a low barrier for entry for analysts
  - Can provide an immediate benefit in knowledge transmission within an experiment
Other technical areas of work

**Conditions Data**
- Growth of alignment and calibration data is usually linear in time
  - Per se, this does not represent a major problem for the HL-LHC
- Opportunities to use modern distributed techniques to solve this problem efficiently and scalably
  - Cacheable blobs accessed via REST
  - CVMFS + Files
  - Git

**Visualisation**
- Many software products developed for event visualisation
  - Part of the framework, with full access to event and geometry data
  - Standalone as a lightweight solution
- New technologies for rendering displays exist, e.g., WebGL from within a browser

**Security**
- We have a large infrastructure that is an important resource for us
- Evolution of authorisation and authentication away from X.509 towards simpler mechanisms
  - OAuth used widely now
- Enhancing effective security incident response teams

- These areas are examples of where we can refocus current effort towards common software solutions
- This should improve quality, economise overall effort and help us to adapt to new circumstances
Software Development - Process and Tools

- **Experiments have modernised their software development models a lot recently**
  - Source code has migrated, by and large, to git
    - Far more developer independence and flexibility than before
  - Social coding sites like github and gitlab amplify these advantages considerably
    - Pull/Merge request workflows help a great deal with code quality
    - Continuous integration and code review become natural and much easier than before
    - Enables widespread collaboration across many boundaries of geography
  - CMake is becoming a pretty standardised way to build
  - This is a suite of common tools that facilitate collaboration and knowledge sharing

- **Additional tools would benefit the community:**
  - Static analysis of code, refactoring code, performance measures
  - As well as a more regular generic development forum
Training and Careers

● Using new tools requires investing in training for the community
  ○ The more commonality in the tools and techniques, the more training we can share
    ■ ALICE and LHCb recently did this in practice using the StarterKit material
  ○ This provides preservation and propagation of knowledge
  ○ A lot of the training we need to do is generic, but some is quite specific (to HEP or experiment)
    ■ We should also encourage appropriate training at the undergraduate and graduate school level

● Our environment is becoming more complex; we require input from physicists whose concerns are not primarily in software
  ○ Sustainability of these contributions is extremely important

● Recognition of the contribution of our specialists in their careers is extremely important
  ○ There needs to be an appropriate career path for software experts as much as any other technical discipline on which our success depends
  ○ We should also improve our publication and citation record (weak in some areas) and explore new avenues, e.g., Zenodo
Parallelisation - Promising Directions

● Describe *what* you want to do, not *how* to do it
  ○ Leave that for the backend
  ○ Can parallelise much more easily and reorder calculations for maximum efficiency
  ○ Lazy evaluation helps optimise the workflow graph and will cache results
  ○ Approach extends more easily to new backends and facilities
    ■ Inspired by, e.g., Apache Spark

● Use different parallelisation models
  ○ Message passing models are conceptually easier and have less thread safety problems
    ■ ALICE O2 approach or the new Gaudi Functional model
    ■ Better adaptation to offloading to different devices
  ○ *ML toolkits are generally good at this* (e.g., TensorFlow)
Vectorisation and Cache Hierarchy - Promising Directions

- Exploiting vector registers is frustrating
  - Many different vectorisation models (SSE4.2, AVX, AVX2, AVX512, NEON, SVE, AltiVec)
  - Auto-vectorisation from the compiler is generally fragile and hard to use
  - Best to use an abstraction library: VecCore
  - Add fundamental vector types to C++
  - Optimise code at compile time for different backends

- Memory Layout
  - Efficient use of vectors requires also efficient load and store
  - Underlying storage of ATLAS xAOD is vector friendly
  - AIDA PODIO does this same for a simple EDM
  - Even C++ evolution, like range_v3, can support views of complex vector types
Advancing from here

- Community White Paper process has been a success
  - Engaged more than 250 people and produced more than 300 pages of detailed description in many areas
- Summary roadmap lays out a path forward and identifies the main areas we need to invest in for the future for our software upgrade
  - Supporting the HL-LHC Computing TDRs and NSF S2I2 strategic plan
  - You can still sign :)!
- HEP Software Foundation has proved its worth in delivering this CWP Roadmap
  - Achieving a useful community consensus is not an easy process
  - Sign up to our forum to keep in touch and get involved (hep-sf-forum@googlegroups.com)
- We now need to marshal the R&D efforts in the community, refocusing our current effort and helping to attract new investment in critical areas
  - The challenges are formidable, working together will be the most efficacious way to succeed
  - HSF will play a vital role in spreading knowledge of new initiatives, encouraging collaboration and monitoring progress
  - Next HSF workshop in March, shared with WLCG, should start to put our ideas into practice:
    - C++ Concurrency, Workload Management and Frameworks, Facilities Evolution, Analysis Facilities, Training, ...