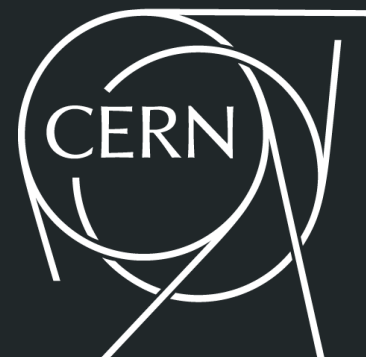




HEP Software Foundation Community White Paper

Graeme Stewart, CERN EP-SFT

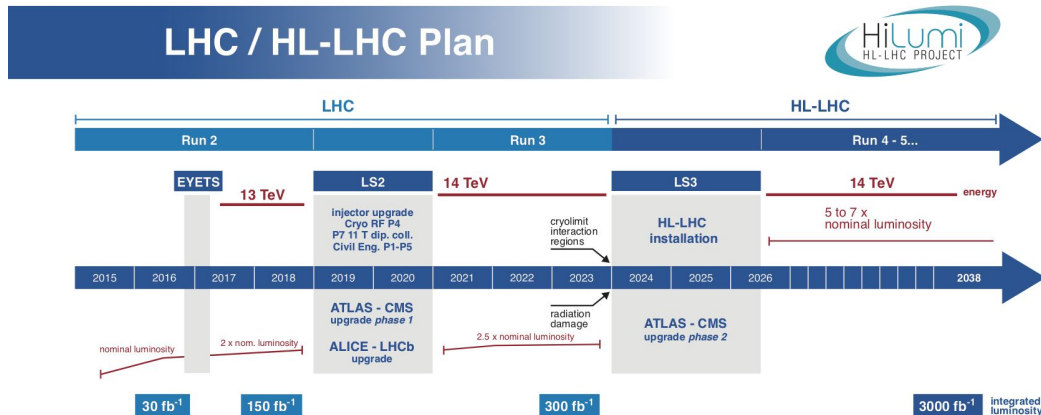


Experimental Particle HL-LHC and Intensity Frontier

Our mission:

- Exploit the Higgs for SM and BSM physics
- b, c, tau physics to study BSM and matter/anti-matter
- Dark matter
- Neutrino mass hierarchy, CPV
- QGP in heavy ion collisions
- Explore the unknown

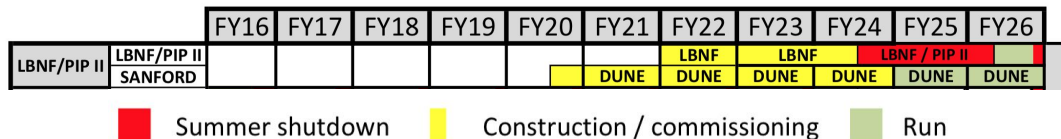
We support this physics program with a very large (50M+ SLOC) software ecosystem and the WLCG infrastructure



FNAL Intensity Frontier

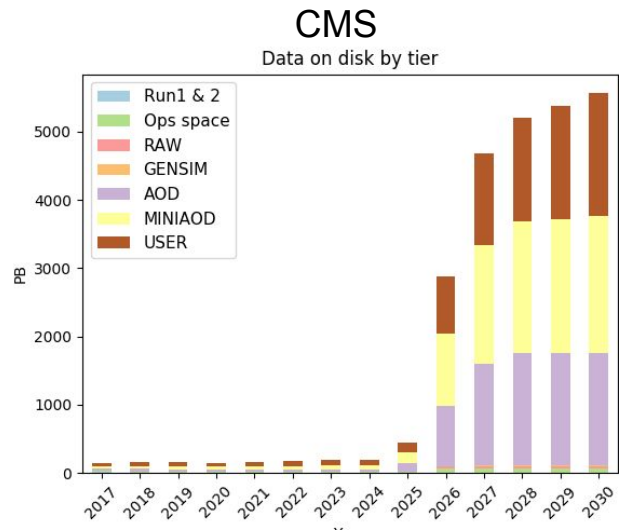
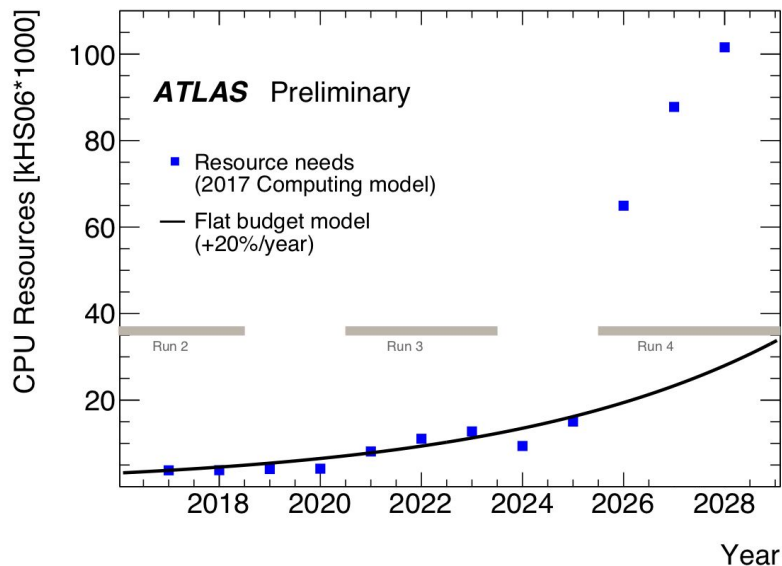
Fermilab Program Planning
20-Feb-17

LONG-RANGE PLAN: DRAFT Version 7a



Software and Computing Challenges

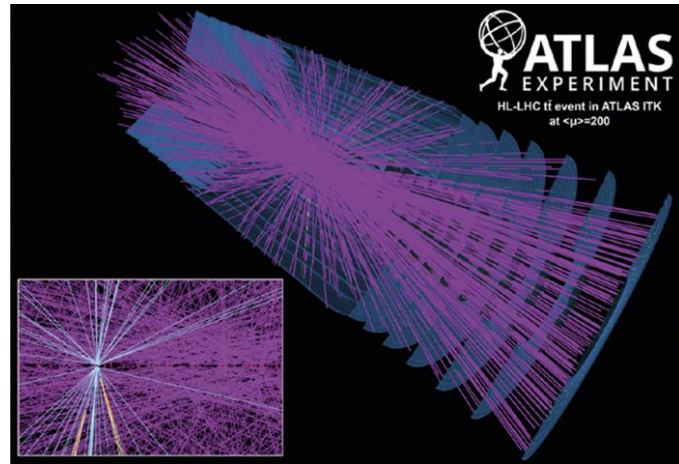
- HL-LHC brings a huge challenge to software and computing
 - Both event rate and complexity rise



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

Software Challenges for HL-LHC

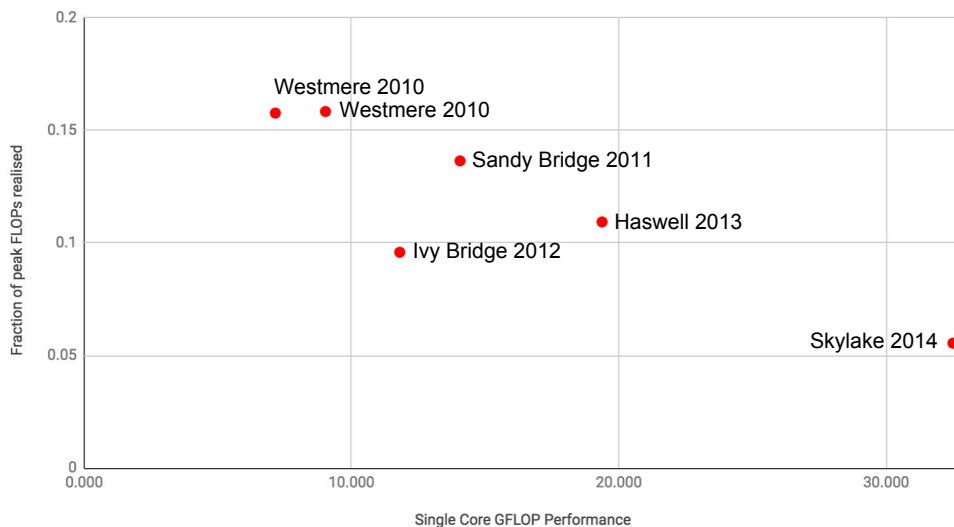
- Pile-up of $\sim 200 \Rightarrow$ particularly a challenge for charged particle reconstruction
- With a flat budget, Moore's lawish improvements are the real maximum we can expect on the HW side
- HEP software typically executes one instruction at a time (per thread)
 - Since ~ 2013 CPU (core) performance 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

Geant4 Simulation



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-ocracy*

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)

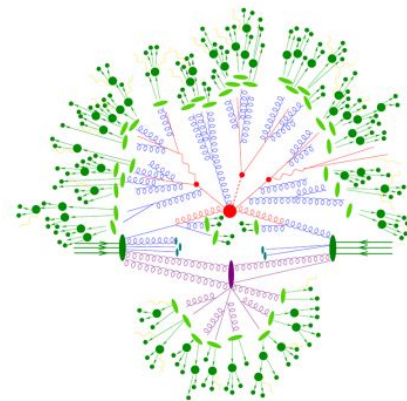
A Roadmap for HEP Software and Computing R&D for the 2020s

- 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

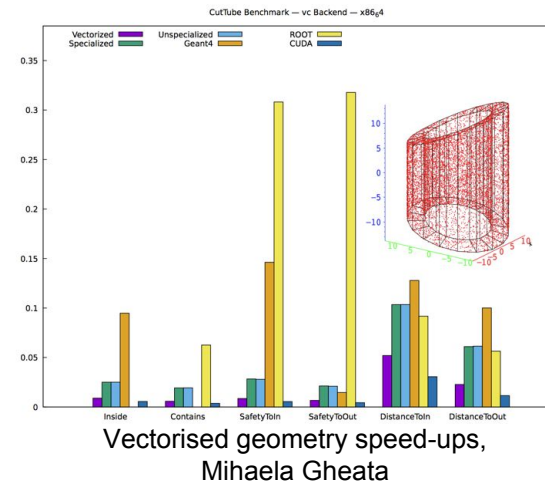
Detector Simulation

- **Simulating our detectors consumes huge resources today**

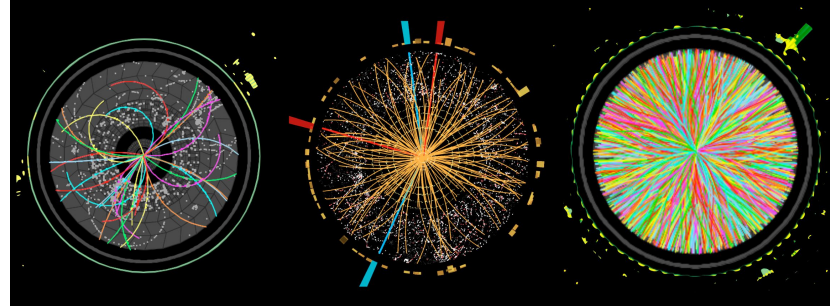
- Remains a vital area for HL-LHC and intensity frontier experiments in particular

- **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 modelling**
 - 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

Data Analysis and Interpretation

- **Today we are dominated by many cycles of data reduction**

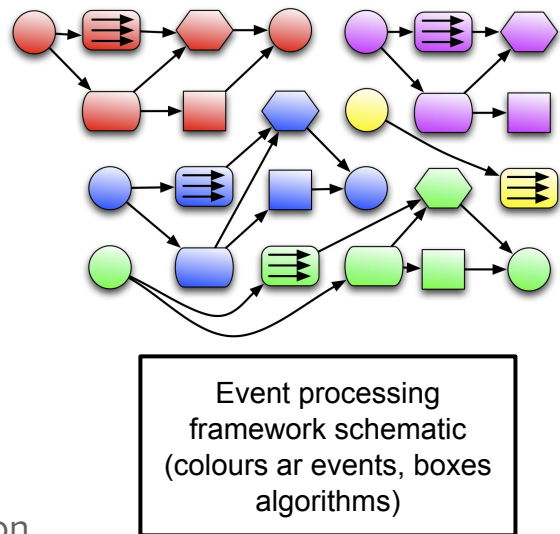
- Aim is to reduce the input to an analysis down to a manageable quantity that can be cycled over quickly on ~laptop scale resources
- Key metric is 'time to insight'

- **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**
 - **Adaptation 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?**



Other technical areas of work

Conditions Data

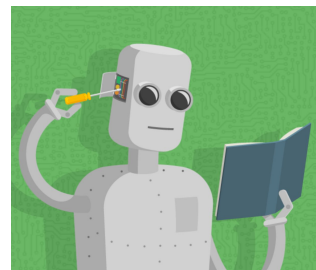
- Growth of alignment and calibration data is usually linear in time
 - Per se, this does not represent a major problem for the HL-LHC
- Opportunities to use modern distributed techniques to solve this problem efficiently and scalably
 - Cacheable blobs accessed via REST
 - CVMFS + Files
 - Git

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

- 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

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), enhanced training methods, and community-supported (Python) packages
 - 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

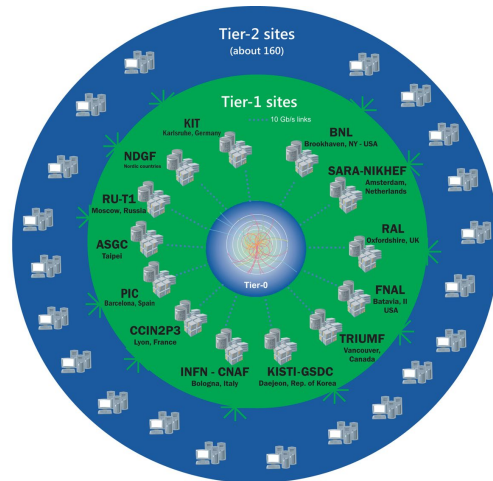
Data Management and Organisation



- **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



Security Matters



- We have a large infrastructure that is an important resource for us
 - Protecting is necessary for both our work and for our reputation
- Trust and policy
 - Evolve away from “in HEP house” to modern data exchange
 - Support integration of commercial resources and hybrid clouds
 - Need to comply with new legislation, e.g., EU Data Protection
- Operational Security
 - Better intelligence sharing for threat monitoring and response
 - Broaden regional participation
 - Coordinate with other communities, R&E Forum for incident response
- Authentication and Authorisation
 - Generic authentication services (e.g., eduGAIN) help users and are easier than X.509
 - Authorisation still needs to be in HEP control (VO management)

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

Software development, training and careers

- **Experiments have modernised their software development models a lot recently**
 - Moving to git and CMake as standard components
 - Using social coding sites (gitlab, github) coupled to Continuous Integration
 - **Additional tools would benefit the community:** Static analysis of code, refactoring code, performance measures, **re-establishing the development forum** (*a la* Concurrency Forum)
- **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
- **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**
 - We should become better at publication and citation of work to help this (and use new tools like [Zenodo](#))

Advancing from here

- **Community White Paper** process is **concluded** 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, ...