# Updates on Software and the HEP Software Foundation

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LHCC Referee Meeting 1.3.2016

### What's ahead of us?

- Increasing complexity and multiplicity of physics events a challenge for simulation and reconstruction performance
- The free lunch is over (no news!) and we have to actively address problems of SW performance
- Have to re-learn many things due to evolution of CPUs and new architectures arriving
- Do not have the resources to evaluate every new technology in each experiment independently
- Have to seek commonality and collaboration in new developments resulting from the evaluations

⇒ Improve both on SW efficiency and efficient usage of people's time

### **Current Status and Activities**

- HEP Software Foundation (HSF) as the umbrella for addressing these problems together!
  - Collection of ideas and proposals in 2014 and startup-team formed
  - Kick-off workshop Jan 2015 at SLAC

#### Sharing expertise

- Schools, trainings and courses (not always easy to find), wikiToLearn
- HEP S&C Knowledge Base
- HSF Technical notes
- Topical fora and working groups in the HSF

#### New hardware architectures and technologies

- Concurrency forum
  - Evolving into a general software technology forum
- Usage of resources provided on best-effort basis by e.g. CERN's TechLab / Openlab
- Porting to new architectures efforts within the LHC experiments

### Current Status and Activities II

#### Software performance

- Simulation: parallelisation of Geant4; <u>GeantV</u>
- Reconstruction: HSF common tracking SW forum + <u>Machine</u>
   <u>Learning Forum</u>
- I/O: parallel ROOT I/O, key-value-store evaluations
- Mathematics: MetaLibm
- Ad-hoc improvements and parallelization in various SW projects
- Performance tools (e.g. <u>igprof, FOM tools</u>)

#### Supporting developers and participating projects

- Providing best practices to facilitate integration into HEP ecosystem
- Project templates for bootstrapping new projects
- Development services
- Help in selecting the proper SW license
- Quite some activity in HSF, even though participation in the startup-team is on volunteer/best-effort level

# HSF Activities and Working Groups

Working Group	Objectives	Forum - Mailing list
Communication and information exchange	Address communication issues and building the knowledge base Technical notes	hep-sf-tech-forum
Training	Organization of training and education, learning from similar initiatives	hep-sf-training-wg
Software Packaging	Package building and deployment, runtime and virtual environments	hep-sf-packaging-wg
Software Licensing	Recommendation for HSF licence(s)	hep-sf-tech-forum
Software Projects	Define incubator and other project membership or association levels. Easy-start project templates	hep-sf-tech-forum
Development tools and services	Access to build, test, integration services and development tools	hep-sf-tech-forum

# **HSF** Topical Fora

### Software Technology Forum

- Technical issues to embrace new technology in our software
- Ongoing activity

### Reconstruction Algorithms Forum

 All matters of event reconstruction and pattern recognition software; 3 in-person meetings

### Machine Learning Forum

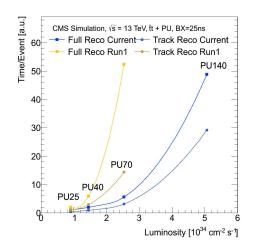
- ML discussions and code development in the context of HEP
- Development of relevant tools, methodology and applications

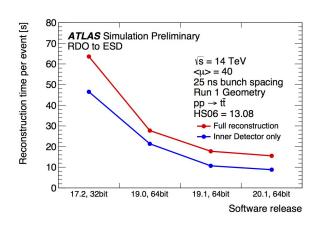
## **Cross-experiment Collaborations**

- There are quite a few (more or less) new cross-experiment collaborations, with involvement or moderation of the HSF - going beyond WLCG
- Experiment frameworks
  - Gaudi (ATLAS, LHCb, FCC)
  - FAIRRoot (FAIR, ALICE)
- Common Conditions Data Project
  - Discussion/cooperation between ATLAS, Belle II, CMS and LHCb
- Common Software Build and Packaging Tool efforts
  - Working group of HSF comparing HEP and non-HEP solutions
  - Starting point was LCG's Librarians and Integrators Meeting
- Cooperation on Reconstruction Software
  - "Connecting the Dots" tracking workshop extended by HSF session about common tracking implementations
- AIDA2020 (EU funded)
  - DD4hep for detector description (LCD, FCC, potentially LHCb)
  - PODIO data model library (FCC, LCD, potentially LHCb)
- **DIANA (Data Intensive ANAlysis)** (NSF funded)
  - 4-year project on on analysis software, including ROOT and its ecosystem

# (Physics) Code Optimization

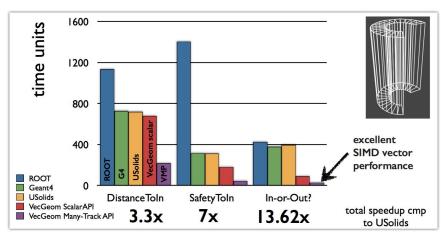
- During LS1 all experiments invested heavily in improving their software
  - Required detailed expert knowledge rare
    - Important to invest on the right topic
  - Significant gains achieved
- One example ATLAS and CMS Tracking
  - Better/vectorized implementations of calculations
  - Adressing hot-spots, e.g. magnetic field in ATLAS
  - Tuned reconstruction strategy for higher pileup,
     e.g. new seeding algorithms in CMS
  - Up to x4 improvements in speed
- Gained expertise fed back into community
  - Ongoing efforts to make improved tracking code available to the wider community
- Tracking performance will stay an important topic for HL-LHC





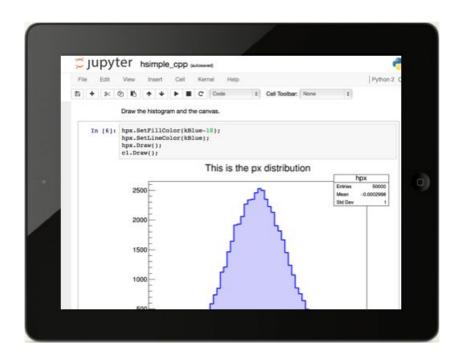
# Preparing Simulation for the Future

- Detector simulation with Geant4 is one of the essential ingredients
  - It is the largest (50%) single consumer of the WLCG cycles.
- Geant4 has been (naively) parallelized with Geant4 Version 10
- The potential of the current Geant4 design for long-term adjustment is limited
  - Software design more than 20 years old (but serves the community well!)
  - Triggered new project GeantV(ectorized)
    - Currently in R&D phase
    - 2016 review milestone is a CMS-like detector
- Necessary revolution of software can even be backported
  - Geometry navigation takes
     30-40% of CPU time in simulation
  - Addressed with new "VecGeom" library in GeantV
  - Substantial performance gains also in scalar mode & Geant4



# New Paradigms arriving

- Software needs to operate well in a wider set of environments
  - Clouds and supercomputers require more flexibility on the application side
- Cloud services not only limited to providing resources and storages
  - Software-as-a-service a very successful model (e.g. webmail, Google Doc)
  - Could extend this to the physics analysis use-case
- ROOT investigating new paradigms
  - Notebook interfaces (Jupyter) for browser-based analysis
  - Declarative instead of imperative data analysis ("the what and not the how")
- Impact and chances for physics analysis workflows yet unclear



# **Backup**

# Support for multiple Architectures

- For many years we have been developing for/running on x86 (Intel) architectures
  - Other platforms mainly for code-checking
- The landscape is much more complex now
  - ARM coming from the low-power consumption market
  - Power8 a common platform in super-computing/HPC environment
  - Dedicated vector processors (e.g. GPUs)

#### Ongoing activities

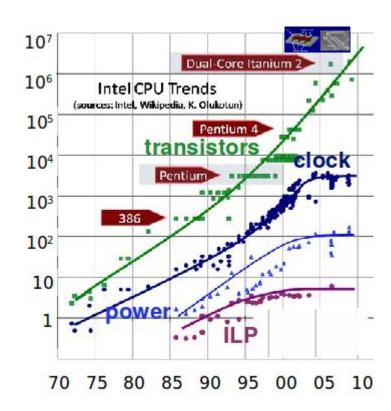
- Projects like Geant4 / ROOT already being tested on a variety of platforms
- CERN IT providing multiple platforms on best-effort basis (TechLab)
- Porting efforts within the experiments
- Concurrency forum

### **HSF** Timeline

- Jan 2014: <u>HEP software collaboration proposed</u>
- Apr 2014: <u>HEP software collaboration meeting</u>
- Spring/Summer 2014: gathering White Papers from the community.
- Oct 1 2014: Startup plan approved and startup team established. Agreement communities and software domains to focus on initially.
- Nov 11 2014: White Paper Analysis and Proposed Startup Plan released, followed by discussions with many parts of the community prior to the SLAC workshop.
- Jan 20-22 2015: SLAC HSF workshop established concrete activities and next steps
- Apr 17, 2015: HSF meeting at CHEP 2015, Okinawa to present progress, assess opportunities emerging from CHEP, and discuss next steps.
- June/July 2015: Intensive discussions in Packaging Working Group
- Sep 2015: <u>Technical Notes</u> policies published more in the queue
- Sep 2015: HSF on WikiToLearn
- Nov 2015: HEP Knowledge Base finished
- May 2016: HSF Workshop in Paris

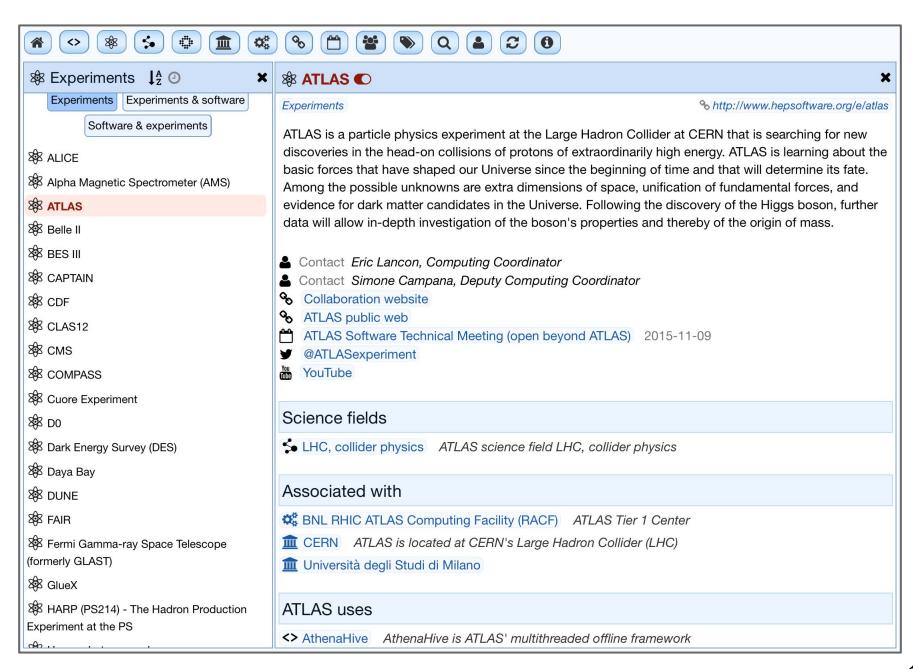
# Stagnation in Speedup

- Performance of our code scales with clock cycle (hence is stagnant!)
- Needs will increase more than tenfold and the budget will be constant at best
- HEP code needs to exploit new architectures and to team with other disciplines to share the optimization effort
  - Data & instruction locality and vectorisation
- Portability, better physics and optimization will be the targets
- Simulation can lead the way to show how to exploit today's CPU's resources more effectively in complex applications



### **Knowledge Base**

- Software catalog, software categories, science fields, community, and events
  - implementation is a browser-based app (javascript client, node.js server, json in between, MySQL)
  - o authentication is via github, google, facebook etc.
  - emphasizes easy adding/editing of content, and extensibility. Adding content should be fun.
- Available at <a href="http://hepsoftware.org">http://hepsoftware.org</a>
  - Comments/feedback are welcome!
  - Just start filling it!
- Implementation based on ATLAS' DKB (data knowledge base)



### Software Packaging

- Topics
  - package building, deployment, runtime environment, new technologies like Dockers, cmake best practices
- Organized a series of discussions/presentations on packaging and build tools (8 meetings)
  - Current practices inside and outside HEP
  - Document to summarize findings being prepared
- Trying a hands-on approach to increase share of actual code even if existing experiments and projects locked-in to a certain packaging solution
  - Common "build recipes" protocol

join the <u>hep-sf-packaging-wg</u>

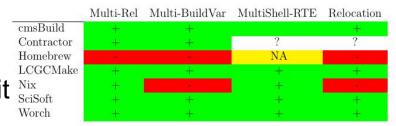
### **Build and Packaging Software Review**

#### Looked at many tools, in particular

 worch, cmsBuild, aliBuild, LCGCMake, SciSoft, contractor (HEP), homebrew, Nix, conda

#### Main problems in HEP software

- reinvention of the square wheel
- non share even within the communit



#### Main problems in non-HEP software:

- non HEP-tools prefer rolling releases / care less about reproducibility
- little support for multi-environment setups

Evolving document available at <a href="https://github.com/HEP-SF/documents/tree/master/HSF-TN/draft-2015-PKG">https://github.com/HEP-SF/documents/tree/master/HSF-TN/draft-2015-PKG</a>

# **Fostering Collaboration**

HSF may have the role of foresting and publicising common software development initiatives. Some examples:

- Next-generation conditions data
  - Belle II / ATLAS / CMS / LHCb
  - 2 meetings: <u>Dec 10</u>, <u>Jan 21</u>
- Track reconstruction
  - Huge challenges ahead
  - Should try to not only share ideas, but concrete code
- Frameworks: Gaudi
  - ATLAS / FCC / LHCb

Satellite projects in the HSF constellation. Examples:

 DIANA (Data Intensive ANAlysis), 4-year NSF funded Focus on analysis software, including ROOT and its ecosystem

### **Technical Notes**

- Technical Notes can be proposals, ideas, whatever people want to add
- First TN with the TN policy has been published
- Some more in preparation:
  - Licence Guidelines, Naming conventions, packaging tools landscape, ...
- Repository and version control in GitHub

TN Number	Title	Authors	Download
HSF-TN-2015-01	HSF Technical Notes policy	A. McNab	PDF GitHub

#### Drafts in the acceptance process:

Draft TN Reference	Title	Authors	Download
HSF-TN-2015-LIC	(Draft) Software Licence Agreements HSF Policy Guidelines	J. Harvey et al.	GitHub
HSF-TN-2015-NAM	(Draft) HSF Platform Naming Conventions - A Proposal	B. Hegner	<u>GitHub</u>
HSF-TN-2015-PKG	(Draft) HSF Packaging Working Group Report	B. Hegner, L. Sexton-Kennedy	GitHub

### Software Licensing

- TN for the HSF Licensing Guidelines is being finalized in the technical forum
  - Plan to publish it this week
- Background information on open source licences approved by the Open Source Initiative
- Set of recommendations for choosing a license and instructions for drafting text to include with the source code

#### THE HEP SOFTWARE FOUNDATION (HSF)

HSF-TN-2015-xx September 17, 2015

### Software Licence Agreements HSF Policy Guidelines

J.Harvey<sup>1</sup>, M.Jouvin<sup>2</sup>, A.McNab<sup>3</sup>, E.Sexton-Kennedy<sup>4</sup>, T.Wenaus<sup>5</sup>

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<sup>5</sup> Brookhaven National Laboratory

#### Abstract

These guidelines were prepared by the HSF Startup Team in order to serve as an aid in establishing a Software Licence Agreement for software projects hosted by the HSF. The report contains background information on open source licences approved by the Open Source Initiative and concludes with a set of recommendations for choosing a licence and instructions for drafting text to include with the source code.

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### WikiToLearn

- WikiToLearn is a wiki-based platform tailored at training and teaching
- Initiated in the context of italian universities
  - Basic idea was that students can improve and extend the material of their professors, while still being qualitycontrolled
- HSF jumped onto that to see whether we can take advantage of it
  - Started adding material to this site
- Now investing in providing interactive tutorials
  - think of the combination of jupyter style notebooks and a privately owned sandbox start tutorial now, resume later (this even triggered a new collaboration w/ the ROOT team)
- This is only the shell, content has to come by the community



# Software Project Templates

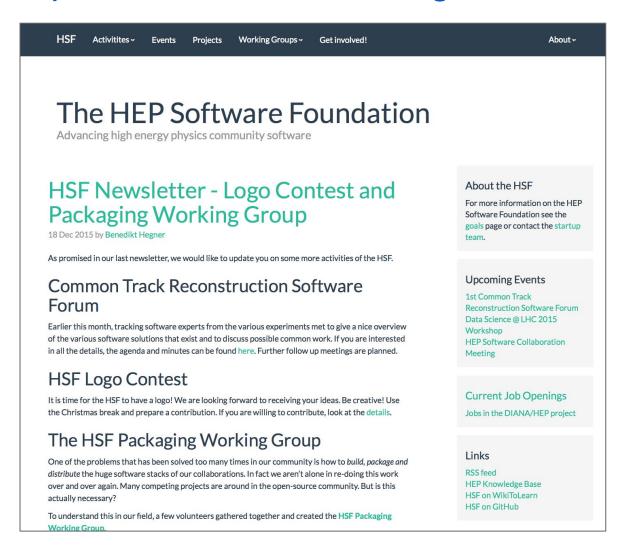
- The idea is to develop a project template implementing these guidelines and best practices
  - For example using the PODIO project (Toolkit for Event Data Models) as guinea pig developed under the AIDA 2020
  - A few more in the pipeline
- Prototype template available at <a href="https://github.com/HEP-SF/tools">https://github.com/HEP-SF/tools</a>
- To support small projects that do not have a collaboration environment available
- To serve as example for shared projects across collaborations
  - reducing impedance mismatch

# Startup Team

- Amber Boehnlein (SLAC)
- Peter Elmer (Princeton)
- Daniel Elvira (FNAL)
- Frank Gaede (DESY)
- Benedikt Hegner (CERN)
- Michel Jouvin (LAL, IN2P3)
- Pere Mato (CERN, co-lead)
- Dario Menasce (INFN)
- Elizabeth Sexton-Kennedy (FNAL)
- Graeme Stewart (Glasgow)
- Craig Tull (LBNL)
- Andrea Valassi (CERN)
- Brett Viren (BNL)
- Torre Wenaus (BNL, co-lead)

### **HSF** Website

http://hepsoftwarefoundation.org



# Some Challenges

#### Status of Technology Tracking

- Future HW architectures
- New technologies/trends worth looking at (cloud based analysis, e.g. Data Mining-as-a-Service?)
- Instrumentation and tools for measuring and improving SW performance
- O What else?

#### Evolution vs. Revolution

- Parallelism / vectorization implies revolutions in our SW
- Challenge to backwards compatibility
- Results of Revolution can still be included as evolution (GeantV's VecGeom as "preview" in Geant4 10.2)

#### Managing available manpower efficiently

- build up more commonality in software projects and procedures
- prepare a common curriculum of development essentials
- provide an easy entry point for people to apply best practices
   (HSF project template + infrastructure to set up + tools)
- improve on quality and ease-of-use of the software we develop (less incentive on reinventing the wheel!)