Report GT 09
Computing, Algorithms and Data
Status and challenges

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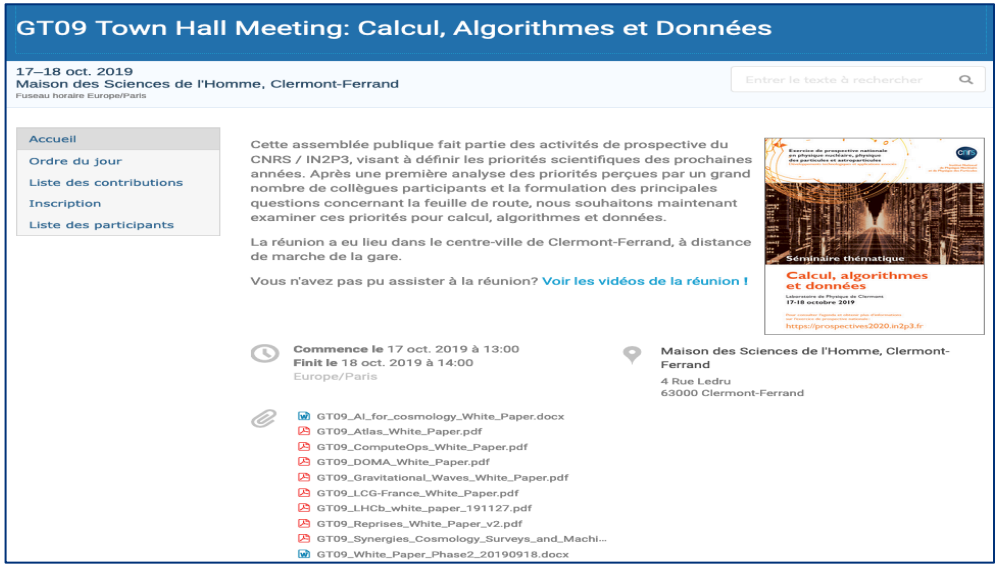
Colloque de Restitution Prospectives IN2P3 GT 09 19-22 October 2021, Giens

Sources for this presentation

- Reports from different groups collected in summer 2019
- GT 09 Town Hall Meeting at Clermont-Ferrand, Oct. 2019



https://indico.in2p3.fr/event/19733/

- GT 09 Summary report (written in 2019)
  - https://box.in2p3.fr/index.php/s/DmJMpRkpdXWcaQY
- Updates from different groups collected in September 2021

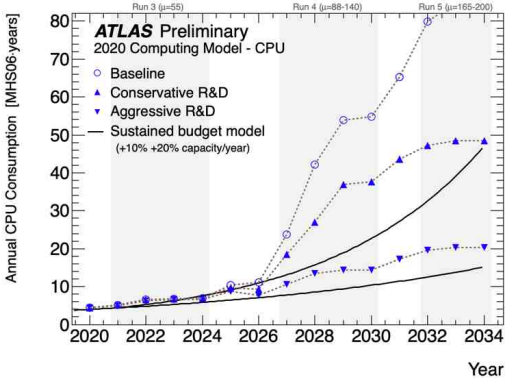
Context

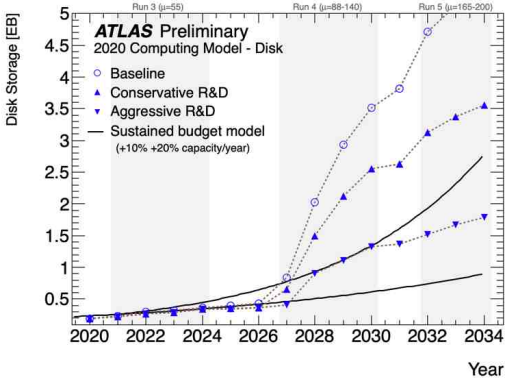
- IN2P3 experiments among the largest producers and users of scientific data
- Our community has produced innovative and disruptive solutions, e.g. WLCG to face LHC challenges
- New challenges in the next decade to meet the very large storage and computing requirements of HL-LHC and of the next generation of astroparticle and nuclear physics experiments

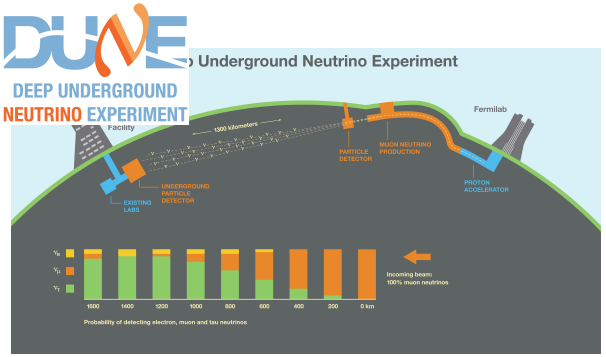
Computing and storage needs

HL-LHC projections

- *Example of ATLAS*



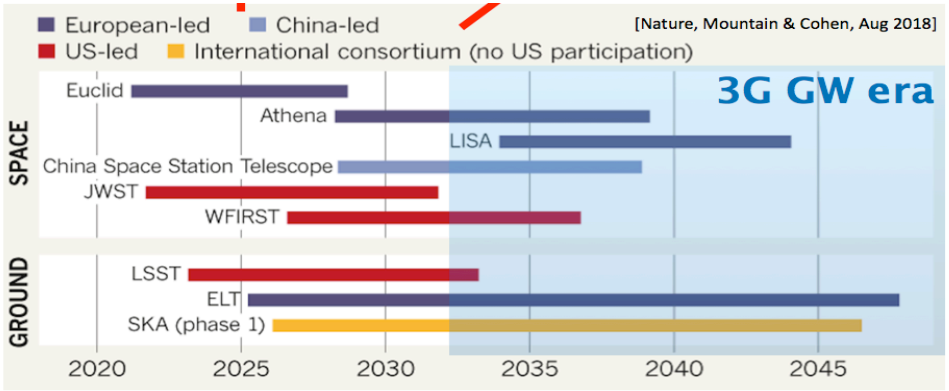




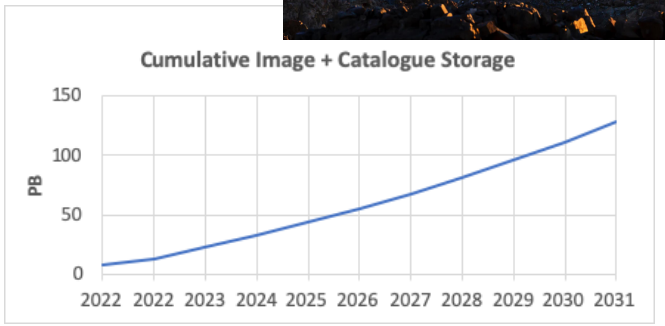
~30 PB/year

Very high computing and storage needs expected in the next decades
Towards the Exabyte era

Astrophysics experiments at 2050 horizon

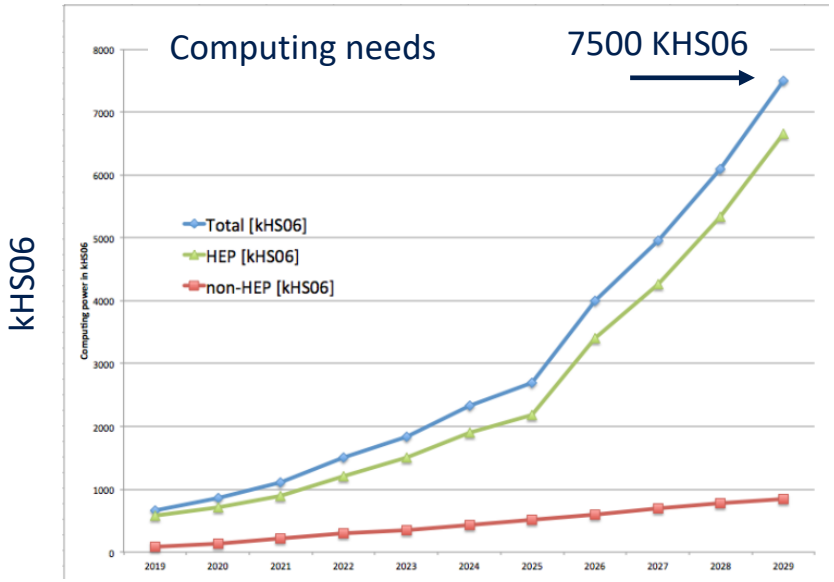


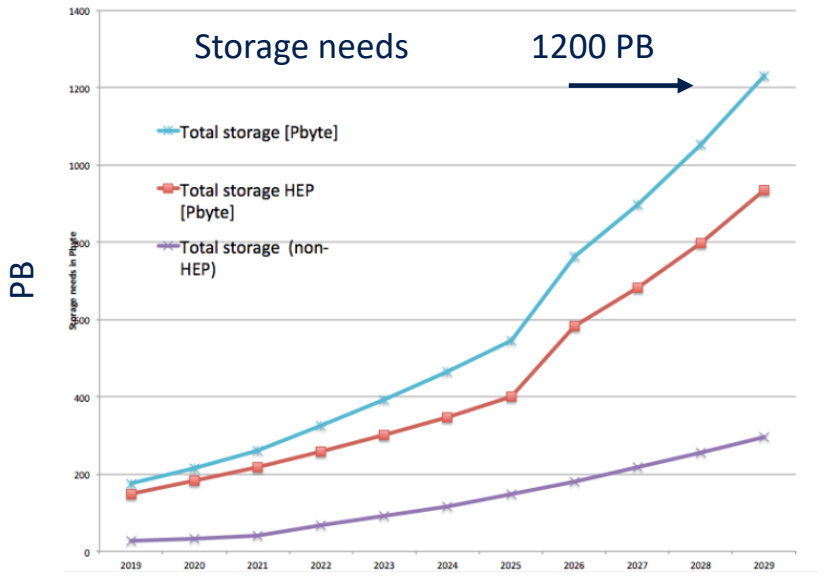
VERA C. RUBIN OBSERVATORY
LSST



Computing and storage needs at IN2P3

- Projections at 2030 horizon





- x10 in CPU power and x6 in storage capacity
  - Not affordable by scaling up computing facilities within a flat budget model
  - Applying incremental changes to the current codes not enough
  - Need to coordinate the efforts with our international partners

Roadmap to face computing and storage challenges

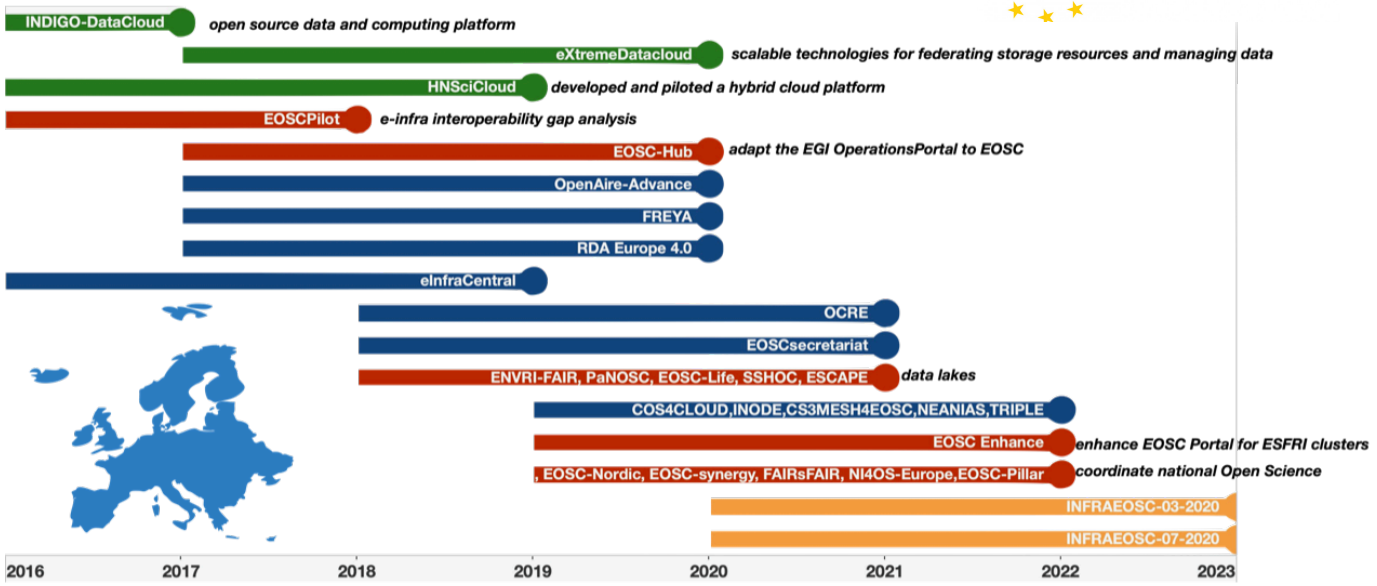
- Adapt the current (grid) e-infrastructure and computing models to make a more efficient usage of resources
- New software development paradigms to make an efficient usage of modern hardware (e.g. SIMD, accelerators)
- Exploit the wide potential of Artificial Intelligence
- Be prepared to the next breakthrough coming with the Quantum Computing
- Enhance software quality assurance
- Training, career development and recruitment strategy

e-infrastructures and computing models
Current situation

- Grid model
  - Computing and storage distributed among hundreds of sites in the world
  - Tier0 at CERN, with a small number of first-class centres (Tiers-1) plus a larger number of centres (Tiers-2)
- CC-IN2P3 as WLCG Tier-1 but also serving other communities (astroparticle, nuclear physics, bio-medical, etc.)
  - Mutualization of services and resources among different experiments to rationalize resource usage and operational costs

e-infrastructures and computing models Evolution

European funded projects related to EOSC



Projects with IN2P3 participation (not directly related to EOSC)
Projects with IN2P3 participation (related to EOSC)
Future projects with IN2P3 participation

DOMA R&D initiated by CERN

- IN2P3 participation within DOMA-FR coll.
- Focuses on data storage and access
- Now in prototyping phase

eXtreme DataCloud

ESCAPE
European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures

Cluster of Astronomy and Particle Physics ESFRI research infrastructures

e-infrastructures and computing models Evolution

- **Proposal of « Data Lake » model as a successor of the grid model**
  - Data would be distributed on much fewer sites with different Quality of Services
    - Remote access (possibly via caches) by analysis and/or simulation centres
    - Heavily relies on the capacity and reliability of the network
  - Reduced human cost for operations
  - Reduced infrastructure cost by exploiting adapted Quality of Services from different storage technologies

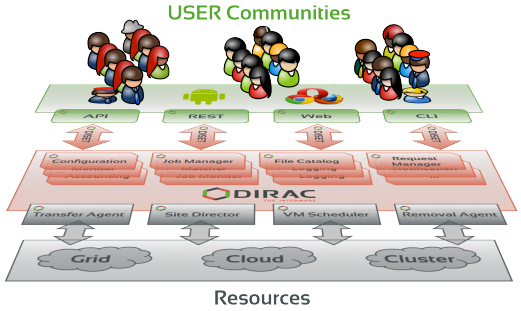
Growing usage of HPC/GPU/Cloud resources

- IN2P3 community traditionally uses HTC resources (grid)
  - Distributing many single-core jobs over thousand cores
- HPC usage steadily growing
  - Framework evolution to support multi-core and/or multi-host (*e.g.* AthenaMP, etc.) applications
  - QCD, magnetohydrodynamics simulations, cosmology n-body, …
- GPU usage rapidly increasing
  - GPU-based algorithms in frameworks (e.g. CMSSW)
  - ML applications
  - Real Time Analysis (e.g. LHCb HL Trigger)
- Cloud computing also increased during the last decade
  - Commercial clouds to absorb production peaks
    - Well adapted to CPU-intensive tasks but not for massive data handling
  - Several Academic clouds (federated in EGI or local platforms)
    - Used as additional resources or to target specific applications

Toward HTC/HPC/Cloud integration for off-line processing

- HPC/GPU infrastructures used today
  - HPC regional mesocenters
  - GPU farm at CC-IN2P3
  - National Jean Zay platform at IDRIS

- Challenges
  - Rationalize usage and access to HPC/GPU centers
  - Provide transparent and efficient access to HPC/GPU and HTC
  - Cope with the diversity of access rules and hardware in HPC centers
- DIRAC@IN2P3 R&D project adresses these challenges



DIRAC is a framework for the **Workload and Data Management** in distributed and heterogenous environments

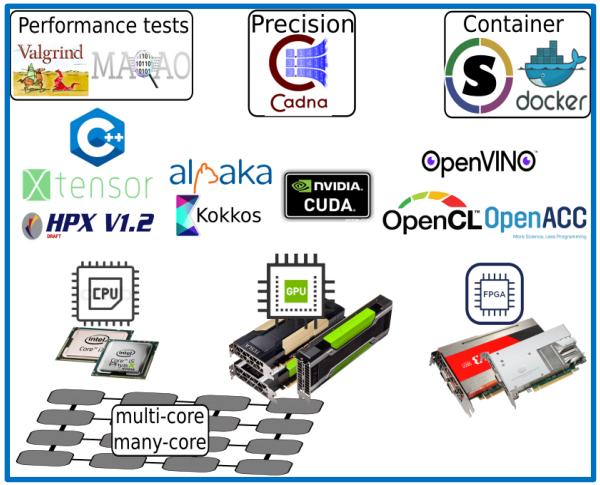
https://dirac.readthedocs.io/en/latest/

Accelerators and Software development

- Need to parallelize our codes at different levels (multi-threading, vectorization, shared memory, GPGPU)
- High potential in reducing computing cost by using accelerators
  - GPU well adapted for highly parallel tasks
- FPGA traditionally used for DAQ, their usage could be extended to
  - Real Time Analysis
  - Optimization of compute-intensive code like analysis or simulation
  - Acceleration of deep neural network inference

Accelerators and Software development

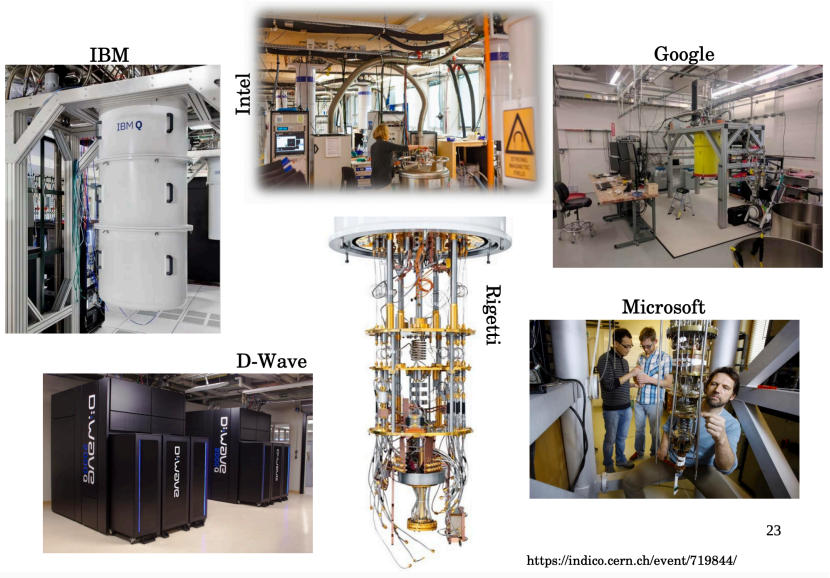
- Challenges
  - Diversity of hardware and plethora of software tools
  - Portability, reproducibility and numerical accuracy
  - The good news is that constructors provide more and more high-level tools targeting different hardware (e.g. nvc++)



- DecaLog R&D project at IN2P3
  - Reprises: Performance, precision and portability
  - ComputeOps: Containers for High Performance Computing
- HEP Software Foundation at international level
- Collaborations with Computer Science community

Quantum Computing

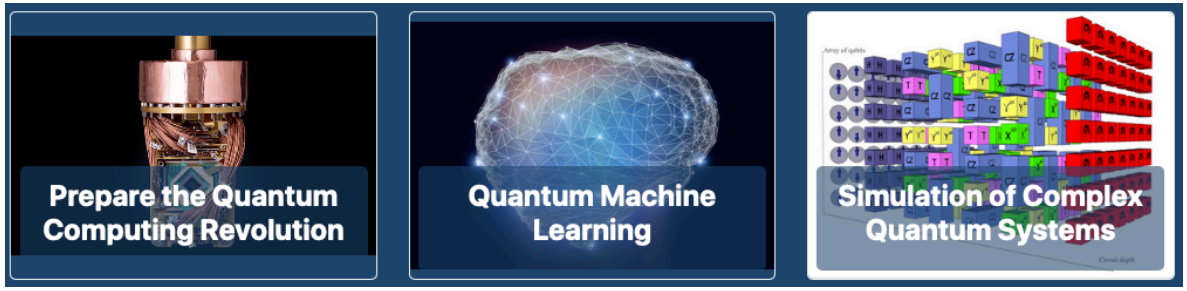
- Quantum Computing is emerging as the next breakthrough by substantially speeding up expensive computational tasks
- First quantum computer demonstrators by D-Wave, IBM, Google, …



- Potential applications at IN2P3 in domains like theoretical or nuclear physics
- **Programming on quantum computers requires to rethink completely traditional algorithms**

Quantum Computing

- Quantum Computing will very likely have little production usage in the next decade but it's an important R&D topic
- **At IN2P3, QC2I R&D project started in Jan. 2021**
  - Collect, within IN2P3, the interests in using quantum technologies
  - Facilitate the access and training on quantum computers
  - Identify pilot applications for nuclear/particle physics and astrophysics
  - Design dedicated algorithms and proof of principle applications
  - Link with similar initiatives within the international community



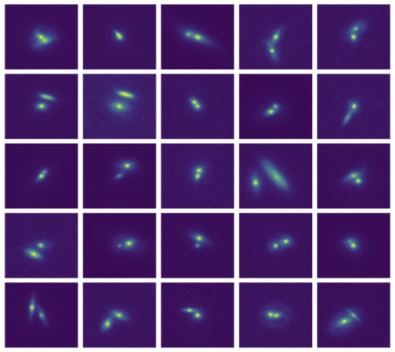
https://qc.pages.in2p3.fr/web/

Artificial Intelligence

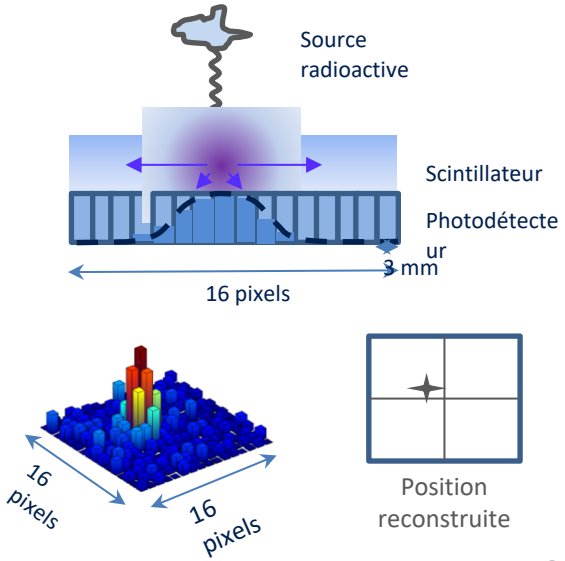
- Machine Learning and Deep Learning already applied in several fields at IN2P3
  - Usage of “traditional” **ML** since many years within IN2P3
  - Some breakthroughs using AI have been achieved (e.g. Higgs boson study)
  - More recently moved to **modern software and algorithms**
  - Lots of **opportunities** with these new approaches

1. Detectors & accelerators
2. Simulation
3. Object Reconstruction, Identification, and Calibration
4. Real Time Analysis and Triggering
5. Uncertainty Assignment
6. Learning the Standard Model – searches for anomalies
7. Matrix Element Method with ML
8. Theory Applications
9. Computing Resource Optimization

ML and DL in HEP



Photometry of blended galaxies with CNNs



Medical Imaging

Artificial Intelligence

- Challenges
  - HEP data are large and have a complex specific structure
    - Not easily handled with ML modern tools, primarily designed for image classification or natural language processing
  - The outcome of AI algorithms must be trusted by the community
  - Importance to open datasets especially for data challenge competitions
  - Increased need of GPU resources
- **Machine Learning R&D project at IN2P3**
- Collaborations with CS/statistician community very fruitful but not always easy to establish
  - Speaking same **language** & getting familiar with vast stat **literature**
  - Question of access to **confidential** experimental data and **authorship**
  - **Publication** in journal of CS/math field is essential
  - Produce outcome **relevant** to CS collaborators

Software quality assurance

- Software quality assurance is essential for long-term code maintainability
- WLCG and spatial projects already impose strict rules for quality assurance
- The challenge is to extend these practices to other IN2P3 projects as a common practice
- Collaborative tools maintained at CC-IN2P3
- Various training actions on software quality during the past years

Training

- Tools and methods become more complex
- Many physicists involved in analysis software development, but only a limited number in core software and R&D projects
- **Training is fundamental to develop the necessary skills and remain competitive at international level**
- Regular training actions organized at IN2P3 since long
  - Ecole informatique, Ecole Statistique, Tutorials at Journées Informatiques, France Grilles and local/regional initiatives, on-line courses
  - Need to encourage a wider participation to help physicists to get more involved in computing and software activities

Career development and recruitment

- Computing and software work is essential for IN2P3 science
  - It should have proper recognition in career development
- Publications as means of academic recognition
  - Currently: regular talks and proceedings at conferences
  - Some publications in specialized journals but the practice is not widespread
- Challenges
  - Attract talented young people
    - Competition for recruitment with industry
  - Keep experienced persons in the field

Conclusions

- e-infrastructure, computing model and software developed by our community allowed for major scientific results during the past years
- New computing challenges in the next decade
  - Require an evolution of the current e-infrastructure and computing model
  - An R&D effort is needed in several areas (software, AI, new technologies, …)
- At IN2P3 several activities already working in this direction
  - Participation to EU projects
  - R&D projects created since a few years under the Calcul et Données DAS
  - Collaborations with Computer Science community
- A list of recommendations in the next talk