GT09: Recommendations for **Computing and data science at IN2P3**

Comité de pilotage

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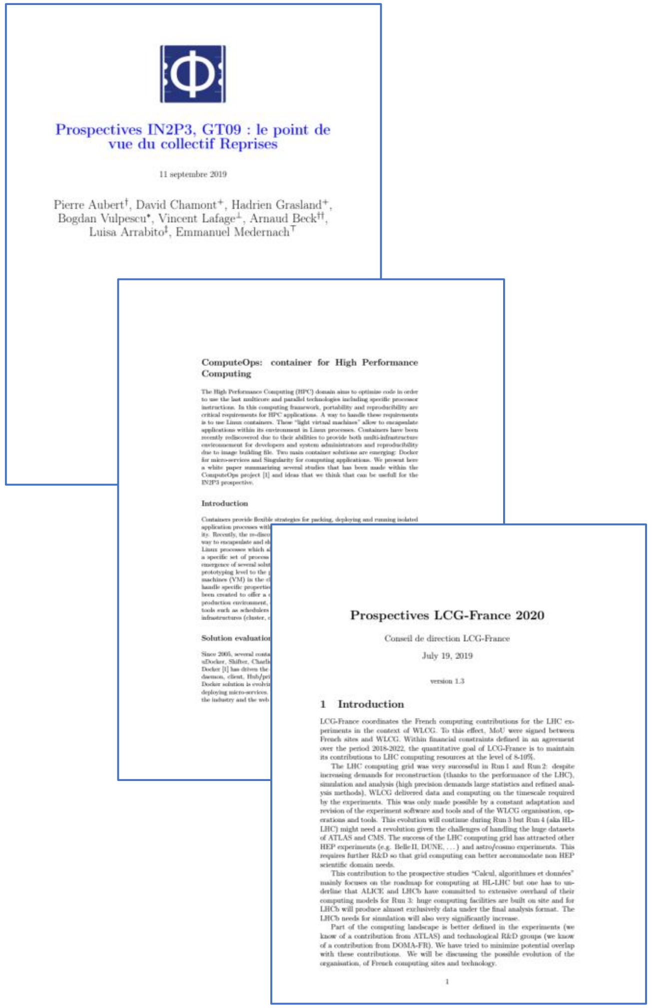
Exercice de prospective nationale en physique nucléaire, physique des particules et astroparticules
Développements technologiques et applications associés

Colloque de restitution de l'exercice de prospective nationale – Giens 2021

Methodology

- July 2019: A community survey to collect feedback (77 answers and 9 white papers received)
  - ✓ Big Data and Cloud Infrastructures, Accelerators and emerging technologies, Internet of Things for Big science, Software and Computing for Atlas, LHCb, DOMA France, Gravitational Waves, Astronomical Survey and Machine Learning, ComputeOps, Reprises, LCG France
- October 2019: Town Hall meeting in Clermont-Ferrand
- September 2021: Updates requested and received
  - ✓ Reprises, ComputeOps, Quantum Computing (QC2I project), LCG France, ATLAS



Prospectives IN2P3, GT09 : le point de vue du collectif Reprises

11 septembre 2019

Pierre Aubert, David Chamont, Hadrien Grasland, Bogdan Vulpescu, Vincent Lafage, Arnaud Beck, Luisa Arrabito, Emmanuel Medernach

ComputeOps: container for High Performance Computing

Introduction

Solution evaluation

Prospectives LCG-France 2020

Conseil de direction LCG-France

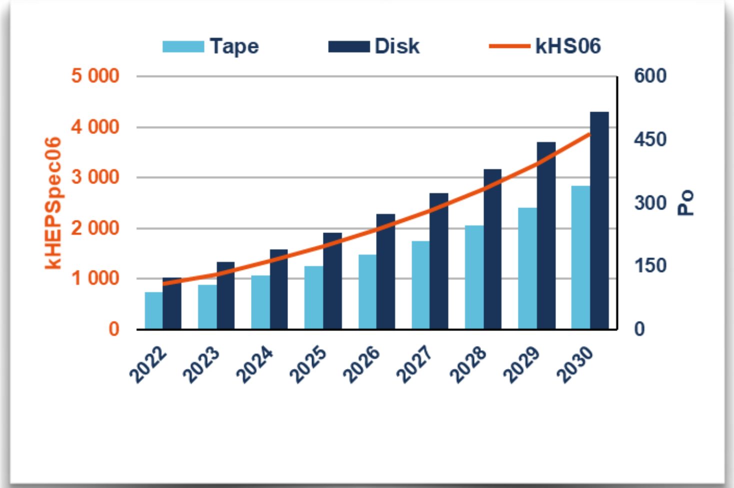
July 19, 2019

version 1.3

1 Introduction

Challenges

- Today, all sciences rely heavily on computing and data science, especially true for the IN2P3 domains
- In the past, our community has proven its capacity to create innovative and disruptive solutions such as Grid computing
- The challenge today is not only the order of magnitude increase of data volume to be expected with HL-LHC but also
  - the growing number of significant data generated in other domains
    - astroparticle, cosmology and nuclear physics
  - the growing needs of diverse technologies



IN2P3 Les deux infinis

Drivers

- Develop a reliable, evolving, and performing e-infrastructure suitable to IN2P3 experiment needs
- Make use and develop breakthrough solutions to tackle the upcoming HEP, astroparticle, and cosmology data flow

➢ **Adapting/evolving IN2P3's computing infrastructure**

➢ **Improving software performance and quality**

➢ **Empowering and strengthening the workforce**

IN2P3's computing infrastructure:
Aim is to preserve a thematic infrastructure

- IN2P3 e-infrastructure is:
  - Integrated in worldwide experiment distributed computing models
  - A Data oriented infrastructure (HTC)
  - Mainly dedicated to permanent production (WLCG, future LSST, …)
  - CC-IN2P3 recognized as a major data centre at the international level
  - ➢ **Allows IN2P3 scientists to play a major role in their collaboration thanks to direct data access**

CCIN2P3

Confirm IN2P3 commitment into a dedicated e-infrastructure to provide efficient IT solutions to worldwide scientific collaborations

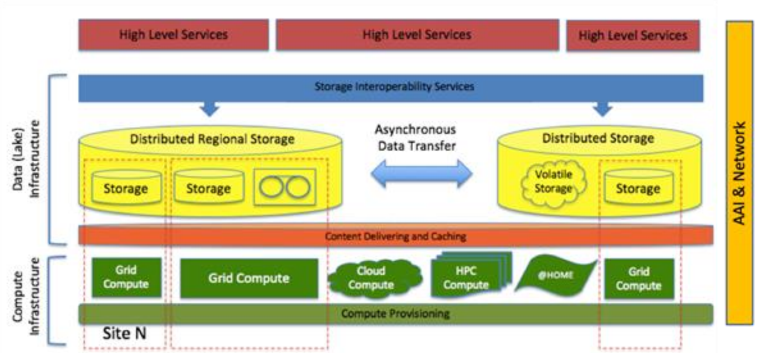
IN2P3's computing infrastructure: Optimise the e-infrastructure organisation

Increase of computing and storage resources constrained by stable funding and Human Resources:

- Dozen of centres with similar features means additional human effort and costs but centralisation implies loss of complementary funding & sites expertise
- Evolution toward a "data lake" model (Access to shared services through a portal and to sites of different natures)
- Participate to international R&D projects like DOMA and H2020 ESCAPE which seek common solutions. Continue to work closely with RENATER.

WLCG
Worldwide LHC Computing Grid

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



Consolidate at the national level the organisation of the resources and services providers, while maintaining the central and stable role of the CC-IN2P3

- Sites could be DATA or CPU oriented
- Federated with a unique user portal

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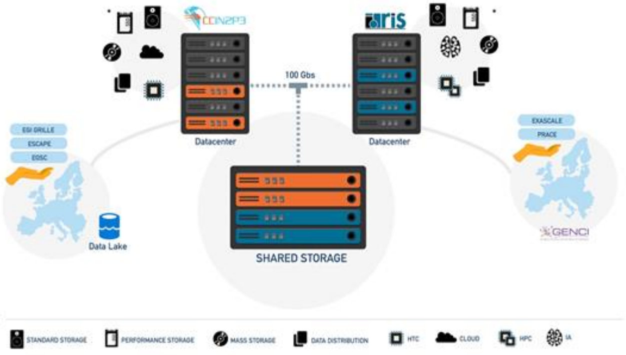
IN2P3's computing infrastructure: Ensure access to new type of hardware

Increase of GPU resource~~s~~ needs due to the growing use of Machine Learning/Deep Learning, both through the multiplication and increasing complexity of applications.

Even if opportunistic usage of GPU in regional HPC centres is increasing their integration is difficult due to their diversity of rules and hardware.



Secure access to large scale GPU resources allowing massive execution of AI and other algorithms, focusing first on the new IDRIS supercomputer platform

IN2P3's computing infrastructure: Improve CC-IN2P3 & laboratories synergies

- CC-IN2P3 experts have a strong experience in production environment and innovative solutions but laboratories, with their tight interaction with scientists could also bring very useful expertise
- Thematic networks play a supporting role by disseminating relevant information especially to smaller communities, organising trainings and resolving technical problems

- Connect experts in thematic networks enhancing their role in advertisement and technical user support.
- Strengthen the links between the CC-IN2P3 and the laboratories for intensified exchanges on user support or innovative solutions

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IN2P3's computing infrastructure
Influence the international decision process

- Major impact of experiment's Computing Models & common tools on IN2P3 e-infrastructure costs and human efforts
- Major collaborations from our community are developing common solutions promoted at the European level by programs like EOSC (European Open Science Cloud)
- Reinforce participation of IN2P3 in such EU initiatives to bring forward proposals that will later positively impact our landscape and the middleware stack.

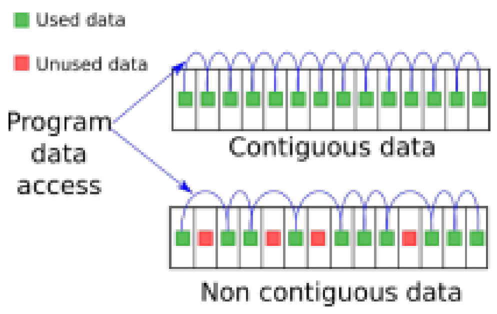
EUROPEAN OPEN SCIENCE CLOUD

Promote IN2P3 engagement in European or international initiatives to enhance our impact on the future computing landscape ecosystem including R&Ds, experiment computing models, choice of common tools across experiments and sites

Software
Improve software performance

Increased data volume and complexity of science problems requires to provide:

- Optimized data model & code
  - rules and recipes, vectorisation, parallelisation, new hardware
  - ensuring sufficient numerical accuracy and maintainable code
- Code portability and heterogeneous environment support to take advantage of new technologies



- Training physicists on data structures and code optimisation
- Strengthening computing engineers and physicists cooperation
- Enhancing the collaboration with the computer science community

Software

Adopt common tools for software development and quality assurance

- Complexity of software
  - requires large team of developers with new skills often distributed worldwide
  - requires automatisation of release & reliability management
  - requires implementation of systematic code reviews

IN2P3-Forge GitLab

Continued effort to provide and release efficient collaborative tools for project management, and the entire DevOps lifecycle

Software

Define and apply common quality standards

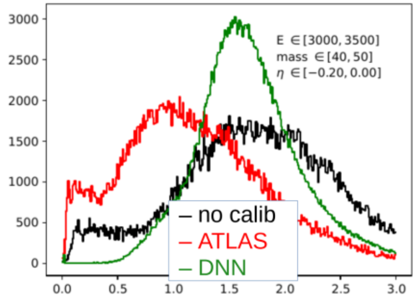
Long-term code maintainability

- New experiment duration prevents from keeping the same team for the whole experiment lifetime for data acquisition to analysis
- Temporary positions (PhD, Post-docs from European contracts) increase~~s~~ expertise loss
- FAIRness challenge requires to have software of good quality, well documented, portable and able to cross decades

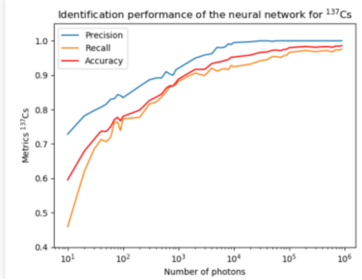
Establish common quality standards at IN2P3 accompanied by reference documents, examples, practical recommendations, guidelines and state of the art good practices

Software

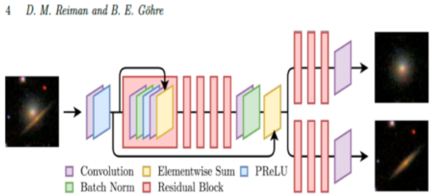
Facilitate Artificial Intelligence usage



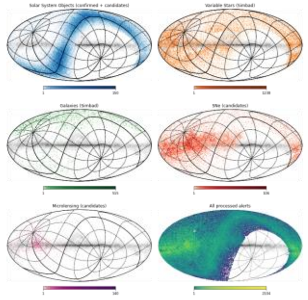
Hadronic jet calibration



Identification of radionucleides



Galaxy deblending



Transient alert classification

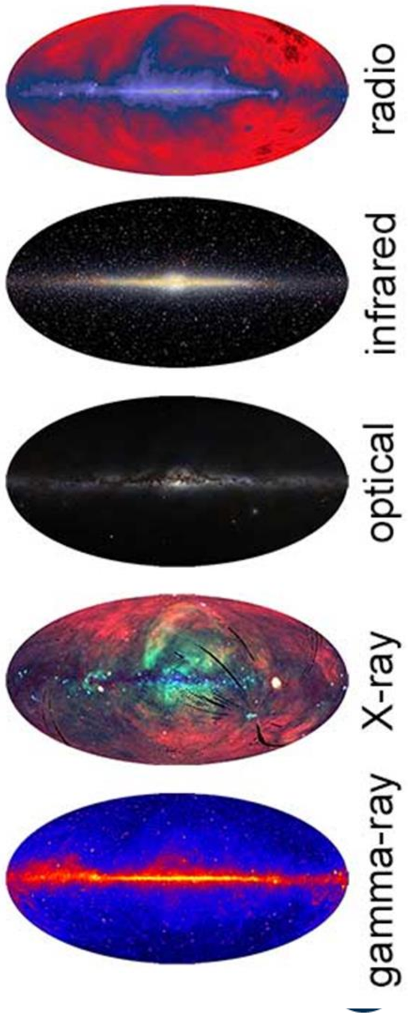
National and international Machine Learning R&D projects increases in all IN2P3 scientific and interdisciplinary domains as HEP, Astro, cosmology, accelerators, …

- Our problems do not easily cast into modern open source tools
  - developed primarily for image classification or natural language processing (Scikit-Learn, Keras, TensorFlow, PyTorch)

Strengthen collaboration with Machine Learning Computer Scientists through the release of open data sets, funding of co-supervised PhD theses, and collaborative projects

Software

Make use of and extend expertise in Real Time Analysis



Real Time Analysis challenges:

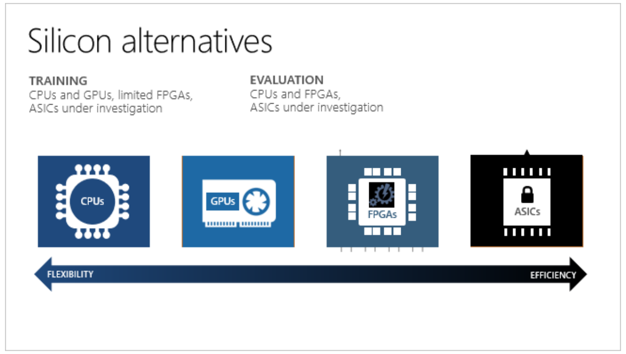
- Launch scientific alerts to the community (e.g. Multi-wavelength)
- Reduce data volume close to the instruments to face Bigdata challenge (LHCb, ALICE, under investigation for ATLAS)
- Monitor science data quality for rapid detector/accelerator adaptation

Require collaborations between electronic & computing experts

- Use in production advanced algorithms on GPU/FPGA to enhance the scientific outcome of experiments, in particular when facing limited storage resources
- Use and extend IN2P3 expertise on Machine Learning/Deep Learning in real-time applications on innovative infrastructures

Software

Engage in evolving and emerging hardware technologies



The increasing computing needs will require to adopt new technologies:

- Better cost/performance ratio including energy savings

For example:

- GPU/FPGA: artificial Intelligence framework focus, Data Centers, New High-Level programming languages
- Quantum Computing: which applications?

- Short term: Continuous follow-up of GPU/FPGA evolutions, identification of possible usage, encourage first testbeds and production installations
- Longer term: Identify the suited applications for Quantum Computing, carry-out a technology survey to acquire the necessary software skills and take advantages of similar initiatives worldwide

Empowering & strengthening the workforce
Ensure an attractive work environment

- **Growing difficulties to keep experienced persons in the field & recruit talented young people**
  - Today non-academic companies are able to propose attractive jobs in the new innovative domains as AI, Data Analytics, Data Scientists based on same technologies we are investigating today
  - Lack of academic recognition for computing work for technicians and engineers as well as physicists
  - Nowadays IT innovations that may attract engineers are no more coming from the research world. The attractiveness of the technology is no longer enough.

Find other levers for career development and attractiveness to ensure the desired skill levels

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Empowering & strengthening the workforce

Lifelong learning

Computing science is moving very fast and the trend is accelerating with major technological breakthrough that requires important learning and personal investments for engineers and scientists

- HPC, data lake,
- Kubernetes, Jupyter notebooks, …
- Artificial Intelligence
- FPGA (requires electronic additional competencies)
- Quantum computing
- …..

kubernetes jupyter docker

Accelerate further training of the workforce in addition to existing initiatives

- through on-line options, such as tutorials, massive open online courses (MOOCs), and webinars

Evolutions since report writing

Improving IN2P3's computing infrastructure

Preserve a thematic infrastructure

- Constant effort

Optimise the e-infrastructure organisation

- DOMA/ESCAPE (actually in test phase)
- Copil Computing platforms

Ensure access to new type of hardware

- FITS EQUIPEX CC-IN2P3/IDRIS
- CC GPU platform

Improve CC-IN2P3 & laboratories synergies

- Computing sciences researchers
- Meetings DAS/LAB/CC

Influence the international decision process

- ESCAPE
- CNRS Shadow committees
- EGI.eu council

Software

Adopt common tools for software development

- IN2P3 Forge & Gitlab
- Decalog

Define and apply common quality standards

- IN2P3 Forge & Gitlab
- Decalog

Facilitate Artificial Intelligence

- Compstat/ML project
- 8 ANR projects
- 24 PhDs/ 8 postdocs

Make use and extend expertise in Real Time Analysis

- Several ongoing project : CTA LHCb…

Engage in evolving and emerging hardware

- FPGA.. THINK project
- Quantum Computing: QC2i

Empowering & strengthening the workforce

Ensure an attractive work environment

Lifelong learning

- School of Statistics
- Online trainings