Review of Software Projects at IN2P3

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IN2P3 Scientific Council, 23rd June 2022

Overview

- Review of software projects with a strong participation of IN2P3
- We present 11 projects from different domains : HEP, astro, nuclear physics, medical physics grouped in 3 categories
  - Simulation
  - Data processing and analysis
  - Workload, data and metadata management
- Not a detailed review
- We will not cover those projects already presented in the thematic sessions

Simulation

- Long-term involvement of IN2P3 in the development of Monte-Carlo simulation software
- Today, 3 main simulation projects around Geant4
  - **Geant4**
    - Toolkit for MC simulation transport of particle in matter
  - **Geant4-DNA**
    - Specialized in the interactions of ionizing radiation with the biological medium
    - Fully integrated in Geant4
  - **GATE**
    - Developed on the top of Geant4/Geant4-DNA
    - Specialized in medical imaging and radiotherapy applications
- Very good synergy among the 3 projects
- Responsibility role of IN2P3 staff with the 3 spokespersons

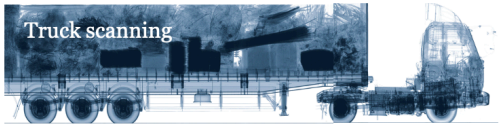
Simulation

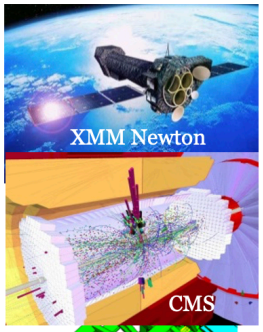
- **nptool**
  - Specialized in the simulation and data analysis of low energy (0-1 GeV) nuclear physics experiments
  - Also based on Geant4
- **Smilei**
  - Simulation of plasmas
  - Using the Particle-In-Cell (PIC) method
  - Massively parallel code

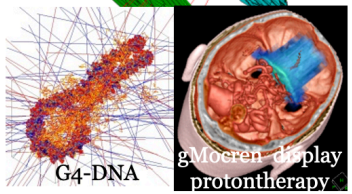
The Geant4 project

Geant4 in a nutshell

- Software toolkit for **Monte-Carlo simulation transport of particles in matter**
  - OO design, written in C++, free, open software
  - https://geant4.web.cern.ch/
- Wide physics coverage
  - Electromagnetic physics:
    - EM « standard » [1 keV – O(PeV)]
    - EM « low energy » [O(100 eV) – O(GeV)]
    - Geant4-DNA down to O(eV) + chemistry phase (free radical transport in water)
    - X-ray & optical
    - Phonons (mK)
  - Hadronic physics:
    - From rest to O(TeV) through
      - string models (high E)
      - cascade ones (intermediate E)
      - Evaporation, capture, etc. (low E)
    - Radioactive decay







- **Used in HEP, Nuclear Science, Medical, Space, Material Science, Homeland Security, etc.**
  - **Mission critical** in many of these areas
- Started in 1994, as the RD44 CERN project
  - Assess interest of OO technologies for particle transport simulation for needs of (future ;)) LHC
  - Alpha version in Apr. 1997, beta one in Jul. 1998
  - **Geant4 version 1.0 Dec. 98**
  - **1st Jan. 1999 : RD44 → Geant4 collaboration**
    - Today: ~130 members, ~30 FTE, 16 Work. Groups
- **Parallel processing** from 2013 with **Geant4 10.0**, with an "event parallelism" scheme
  - Multi-threading processing
    - Ensure all cores have enough memory to run: done by sharing geom. & phys. tables across threads
  - Add flexibility in 2021 with Gean4 11.0 with "tasking"
    - Easier access to hybrid computing as by-product
- **Collaborative & worldwide distributed development model** (GitLab based)
  - With repository and testing infrastructure at CERN
  - Step toward « open development model » this year

The Geant4 project

Challenges

Computing & Physics Performances

- Issue specially acute for HL-LHC
  - **Need factor O(10) speed-up** to fit simulation production in planned HL-LHC computing budget !
  - Need **physics quality to be improved accordingly**
    - to avoid larger (relative) contribution to systematics
- **Strategy:**
  - **Detailed simulation as much as possible**
    - On CPU, with adiabatic evolution
      - When CPU production sustainable
      - Or when no alternative (ie: too complex physics or geom.)
      - And creativity : eg neutron biasing, Woodcock tracking, …
    - On GPU, in hybrid computing workflow
      - **if** current R&D's outcome convincing (news in ~1 year)
        - HEP MC is **evil case** for GPUs ! (issue : divergence)
      - Ongoing GPU R&D's : AdePT (CERN), Celeritas (US)
    - Maybe on other hardware
  - **Fast simulation as much as needed**
    - Classical fast simulation à la GFlash
    - And/or modern fast simulation, **ML-based**
      - EM one & **maybe hadronic one** too
  - **In close collaboration with experiments !**
- On going efforts, HEP-motivated, beneficial to all domains

Risk of Expertise Disruption !

- Many "senior" members were present since the beginning, 28 years ago
- Most of them will have **retired at the HL-LHC start** !
- **Renewal rate too low !**
  - **Brilliant** young members !
  - But with short term contracts…

A new generation of developers is needed !

- Need **new/young members** on the **long run**
- **Smooth transition** must be planned
  - Some expertise **hard to find, specially in physics.**
  - Overlap must be long O(5 years) to become "senior"
- **Conflict** with short term contract policies !
  - An issue all long term projects complain about…
- Working climate & perspectives should be **secure enough**
  - To minimize the risk of loosing people
  - The more talented people, the higher the risk !
- **We alert our funding agencies on the critical need for a new & long term generation !**
  - **This issue is a risk for all Geant4 users !**

The Geant4 project

Geant4 @ in2p3

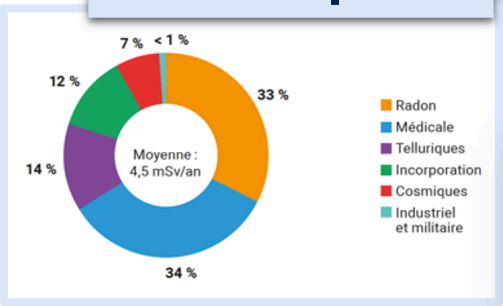
- In2p3 involved in Geant4 since the beginning
  - Started with Michel Maire, LAPP (now retired but still active in G4) an historical developer of EM physics
  - Then joined for fast simulation infrastructure
  - And visualization, analysis
  - …
- In2p3 members have quite **responsibilities** in Geant4:
  - See Steering Board page
  - Responsibilities in Working Groups:
    - Electromagnetic Physics :
      - Largest WG (5 coordinators)
      - **Sébastien Incerti** coordinator for DNA part
    - Generic Processes and Materials :
      - Holds in particular Fast Simulation & Biasing
      - **Marc Verderi** coordinator
    - Novice and Extended Examples :
      - Key entry point for new users and source of "how to"
      - **Ivana Hrivnacova** coordinator
    - For information: Visualization:
      - Laurent Garnier coordinator, was in LAL, moved to Irisa
  - Management:
    - **Marc Verderi**, reelected spokersperson in May this year
      - Second 2-years mandate
    - Was deputy spokesperson for 10 years before
- Geant4 at in2p3 is « Geant4-core » and « Geant4-DNA »
  - DNA part of the Geant4 development cycle and distribution
  - G4-DNA is also a collaboration, driven by Sébastien Incerti
- **Current and to be pursued activities at in2p3:**
  - LP2i Bordeaux:
    - Low energy EM physics and Geant4-DNA
      - Note this includes **GPU usage** for the transports of chemical species in water after the irradiation phase
    - **Sébastien Incerti, Zhuxin Li (thesis), Claire Michelet, Hoang Tran**
  - IJCLab:
    - Analysis package, visualization, basic and extended examples and geometry
    - **Ivana Hrivnacova, Guy Barrand**
  - LAPP:
    - EM physics validation
    - **Sabine Elle**
  - LLR:
    - Bethe-Heitler 5D gamma conversion model (electrons and muons) inherited from developments in HARPO
    - Biasing (variance reduction) techniques
    - Fast simulation infrastructure & GFlash models
    - **Denis Bernard, Igor Semeniouk & Marc Verderi**
- Yearly Geant4 tutorial in Orsay (PHENIICS + ANF every 2 years)
  - Managed by **Ivana**, + Igor and Marc as lecturers

The Geant4-DNA project

Context: exposure to ionizing radiation

1 mSv/an
Public

Chronic exposure



IRSN (2014-2019)

Increasing dose*

Repetitive medical imaging

UCSF & Harvard MS

~10 mSv / scanner abdomen

>100 mSv
Long-term effects

Space missions

ESA

~2,6 times ISS

ESA

6 months = ~ 160 mSv

ESA

Return trip 6 months:
~ 600 mSv

Radiotherapy

NCC

Major questions in radiation protection

- What are the **biological effects** of **low doses** of ionizing radiation?
- What are the **risks** associated with **high doses**?

*« A major challenge lies in providing **a sound mechanistic understanding of low-dose radiation carcinogenesis** »*
L. Mullenders et al. (2009)

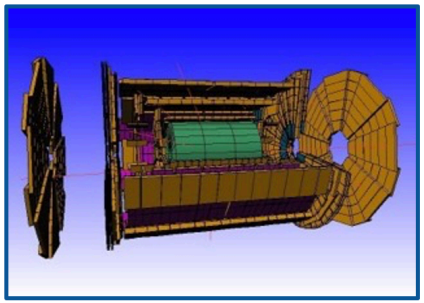
The Monte Carlo approach…

* Equivalent or effective

The Geant4-DNA project

The « Geant4-DNA » project

ATLAS@CERN



geant4.org

Initiated in 2001, based on an idea of the European Space Agency (P. Nieminen)

- To develop the **first open source platform** able to **simulate mechanistically the biological effects of ionizing radiation at cellular scale** during manned space missions

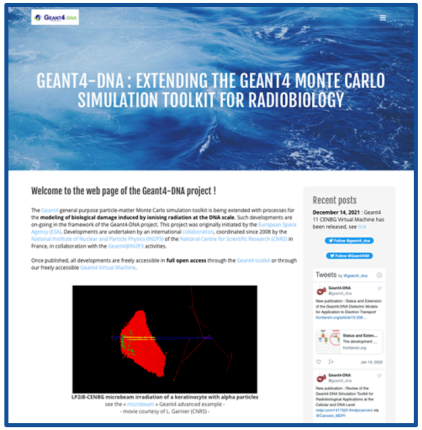
Set of C++ libraries able simulate the different stages of the effects of ionizing irradiation

- Open source, distributable (many OSs), user extensible (OO)
- Radiation **physics** (particle-matter interactions), radiation **chemistry**, radiation **biology**…

Fully integrated in the « Geant4 » Monte Carlo simulation toolkit

- **Ge**ometry **and** **t**racking – version **4**
  - Developed by an international collaboration, initially for the simulation of the large experiments of the LHC at CERN

geant4-dna.org



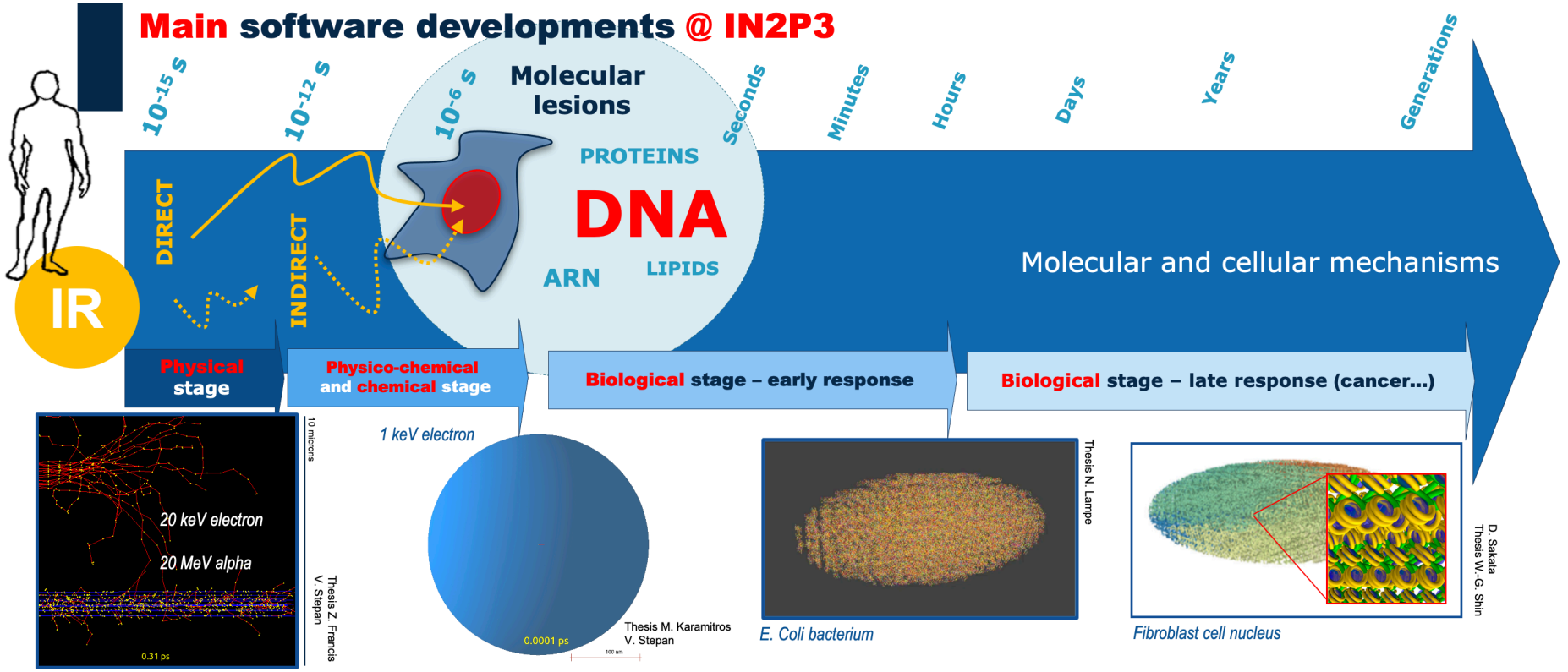
First release of « Geant4-DNA » physics models in 2007

- Step-by-step simulation of particle transport down to low energy (~10 eV) in the biological medium
- **IN2P3** contribution: LP Clermont and LP2i Bordeaux (ex-CENBG)

International collaboration funded in 2008

- ESA proposed to **IN2P3** to lead this collaborative project
- 60 collaborators in 2022 – **13 @ IN2P3** (IPHC, LP2i, LPC, SUBATECH)

The Geant4-DNA project



Simulate « **physical** » **interactions** ($<10^{-15}$ s) with biological matter: **direct** effects and **dissociation** of water molecules.

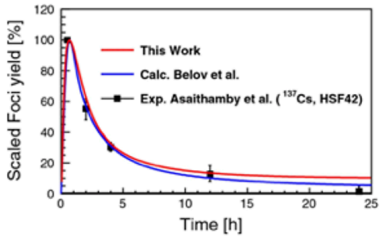
Models describing the **« step-by-step » physical** interactions of **electrons, protons, alpha particles and ions** with biological matter (water, DNA constituents) down to low energy (~ 10 eV)

Simulate « **physico-chemical** » ($<10^{-12}$ s) and « **chemical** » ($<10^{-6}$ s) processes with water molecules in the biological environment: creation of numerous molecular species (e.g. °OH) that cause **indirect effects** on DNA

Alternative approaches to model radiolysis: Steb-by-step, Independent Reaction Time

Simulate **early DNA damage** and its **repair** following physical, physico-chemical and chemical steps (min - h) in biological targets.

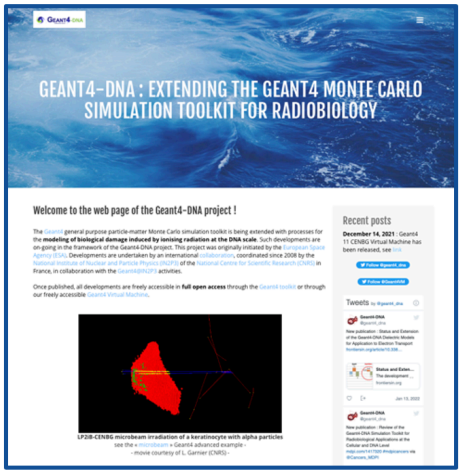
- **Multi-scale geometries** of biological targets
- **Complete simulation chain** for early damage quantification in bacteria and cells
- **Repair** models



DSB foci repair as a function of time

The Geant4-DNA project

Scientific production and animation



All details at:

geant4-dna.org

> 120 publications & open source code (geant4.org – 2 Geant4 releases per year)

Key contributions by young researchers

- 14 PhD **theses** (radiation physics – chemistry – biology) including 13 supervisions/co-supervisions by IN2P3
  - Funding: Bordeaux U., Paul Sabatier U., Conseil général de l'Allier, IRSN, ANR, AUF, CSC Chine
- 17 **postdoctoral** fellows
  - Funding: IN2P3, Bordeaux U., IRSN, AVIESAN, ESA

Regular organization of international conferences, workshops and tutorials

- « **Geant4 at the Physics-Medicine-Biology frontier** » series of international conferences initiated in Bordeaux in 2005
- 4th iteration in Napoli, Italy, on Oct 24th-26th, 2022
- LP2i « **Geant4 Virtual Machine** » (C. Seznec *et al.*): easier access, popular for tutorials

Additional funding

- IN2P3 « collaborative tools »: IRL (South Korea, Japan), IEA (Greece, Lebanon, Serbia), exchanges (JINR, Czech R.), MITI
- Région Nouvelle Aquitaine, Aviesan/Inserm, ANR
- ARC Australia, CampusFrance STAR South Korea, European Space Agency (BioRad1, BioRad2, BioRad3), FNS Switzerland

Permanent recruitments

- 1 IN2P3 research engineer in 2022 @ LP2i Bordeaux: Dr Hoang Tran, now **Technical Coordinator** of the Geant4-DNA Collaboration
- Regular at other institutions: ANSTO (Australia), Campinas (Brazil), Ioannina U. (Greece), IRSN (France), KEK (Japan), NPI (Czech R.) Osaka U. (Japan)

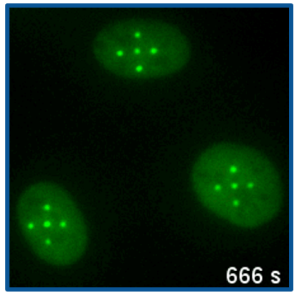
Collaboration led by IN2P3

- IN2P3 re-elected every two years

The Geant4-DNA project

A collaborative program for the next 10 years

... in line with GT10



Ph. Barberet et al. / LP2i

DSB foci
AIFIRA microbeam

Radiation physics

- Extension & improvement of **physics models**: energy / particles / target materials (e.g. solid-state, gaseous)

Radiation chemistry

- « **Mesoscopic** » approach: towards longer times, larger volumes and high dose rates (e.g. Flash RT)
- Experimental **validation** of simulation approaches (SBS, IRT, mesoscopic) with irradiation platforms (e.g. Arronax)

Radiation biology

- A library of **multiscale biological target geometries**: chromatin fibers, plasmids, bacteria, cell nuclei of different lines,...
- Integrated **simulation chains** (physics - chemistry - biology) allowing the prediction of early damage in various lines
- **Repair** models: from early to late effects
- Experimental **validation** of damage (e.g. AIFIRA, Cyrcé, ALTO…)

Computing performance

- **GPU** porting accessible in open source
- **IA**

Medical, space & environment applications

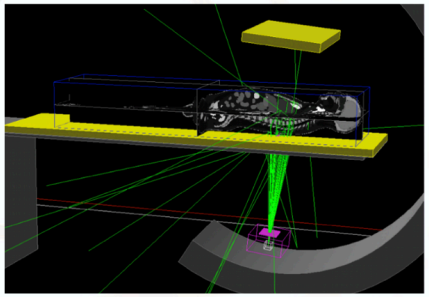
- **Innovative radiotherapies**: internal (new radionuclides, BNCT, …) and external (hadrons, Flash, VHEE, …) – towards risk prediction
- **Space radiation protection** (in coll. with ESA): from incidental spectra to biological damage (e.g. lunar habitat)
- **Environment**: effects of ionizing radiation on living organisms

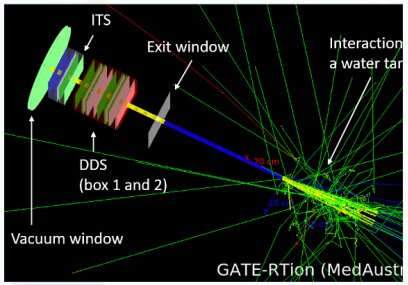
Strategy

- Encourage collaborations with **partners** (INSB, Inserm, CEA, IRSN, etc.) and collective responses to **calls** (Aviesan, Pianoforte, etc.)
- **For the first time, the Geant4, Geant4-DNA and GATE collaborations are led by IN2P3: an opportunity to strenghthen our links?**

The GATE project

a MC simulation platform for medical physics applications





An open source and open access simulation platform for **medical physics**

- **Long term development** based on Geant4 toolkit
- International collaboration composed of **25 members**: laboratories (**6 IN2P3 labs**), companies and clinics
- **Very large community of users** (more than 2000 users)
- **Newly coordinated by IN2P3/CNRS** since 2018
- Funded by regular support from institutions and international calls
- Fruitful involvement in international conferences, workshops & tutorials
  - 2 tutorials /year + Tutorials in medical physics master programs
- High rank and highly cited publications
  - 2 PMB citation prizes in 2009 and 2015 for the 2 collaboration papers

A PLATFORM TO GATHER INNOVATIVE DEVELOPMENTS FOR THE FUTURE CHALLENGES IN MULTI-SCALE SIMULATIONS

The GATE project

The collaboration

25 members, public laboratories and companies developing an open source platform

Spokesperson: Lydia Maigne (LPC)
Technical coordinator: David Sarrut (CREATIS, Lyon)

Research engineer just recruited at LPC for 3 years (IN2P3 funding)

France

- U1101 INSERM, Brest
- IJCLab – CNRS-IN2P3, Paris Saclay
- IRCM INSERM, Montpellier, France
- LPC – CNRS-IN2P3, Clermont-Ferrand
- IPHC – CNRS-IN2P3, Strasbourg
- CPPM – CNRS-IN2P3, Marseille
- UMR5515 CNRS-INSERM, CREATIS, Lyon
- IP2I, CNRS-IN2P3, Lyon
- BioMaps CEA Paris Saclay
- CRCT - U1037 INSERM, Toulouse
- LPSC – CNRS IN2P3, Grenoble

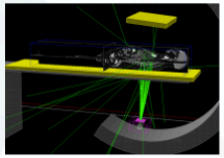
Europe

- Institute of Nuclear Physics Polish Academy of Sciences, Poland
- University of Julich, Germany
- University of applied Sciences, Aachen, Germany
- Medisip, Ghent University, Belgium
- BioemTech, Athens, Greece
- Medical University of Vienna, Wiener Neustadt, Austria
- MedAustron, Wiener Neustadt, Austria
- Christie Medical Physics & Engineering, Manchester, UK
- JPET collaboration, Poland
- Univ. of Patras, Dept of Med. Phys., Greece

Elsewhere

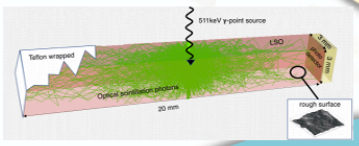
- Memorial Sloan-Kettering Cancer Center, New York, USA
- UC Davis, Davis, USA
- Sogang University, Seoul, South Korea
- QST, Chiba, Japan

The GATE project



DOSIMETRY

- **Interventional radiology**
- **Multimodal nanoparticles** (stem cell therapy on muscle regeneration)
- **Innovative internal RT (177Lu…)**
- CT scan (pediatric applications)
- **Arctherapy**
- SBRT – Interplay effect & EPID
- Database of S-values (OpenDose)
- **GATE/G4DNA micro & nanodosimetry**



PYTORCH

COMPUTING

Neural Networks for:
- Positioning of γ interactions in monolithic PET detectors
- SPECT detector ARF
- GAN for compact beam source modeling

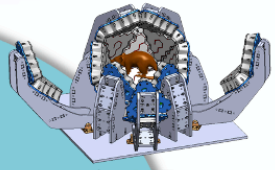
HYBRID SIMULATIONS

PYTHON data analysis

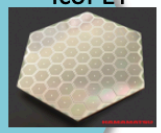
HOT Topics

IMAGING

- Models to define crystal surfaces
- **Optical simulation study on timing performance of monolithic crystals**
- **Testing of new camera and crystal designs**
- **New digitizers for SiPM (analogue and digital)**
- Compton camera
- Proton radiography
- Non-circular orbit motion in SPECT
- JPET (plastic scintillator-based PET)
- Metabolic modeling
- Digital Photon Counting commercial PET



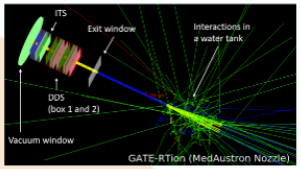
IcoPET



UTOFPET

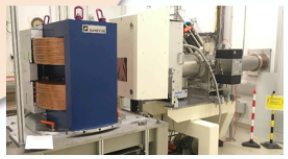
HADRONTHERAPY

- G4 Physics settings
- on-line MR-guidance for particle therapy (integration of magnetic and electric field maps)
- **Neutron dosimetry**
- **Biophysical models for the prediction of RBE ->G4DNA**
- Carbon ion dosimetry and ICRU90 recommendations
- **Range monitoring**
- **FLASH therapy**
- **BNCT & PBCT**



Magnet

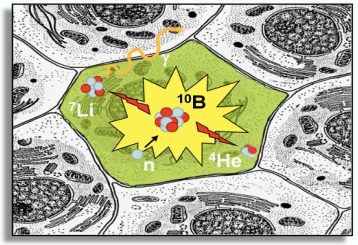
Nozzle

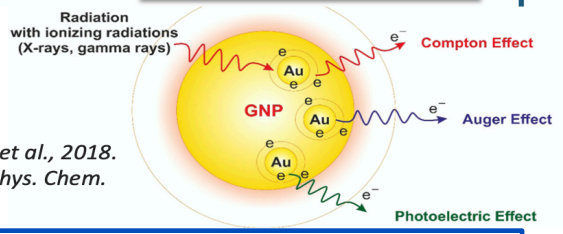


The GATE project

Highlights and future challenges in multiscale simulations

- **Highlights**
  - Validated **quality insurance** of preclinical and clinical beams
  - Reference platform for theranostic treatments
  - Integration and validation of biophysical models to tackle relative biological effectiveness in hadrontherapy
  - New developments to assess **microdosimetry** & **nanodosimetry**
- **Challenges**
  - Improve biophysical models
    - Better combine MCTS simulation outputs to macroscopic simulations
    - Use AI to train the models for different types of cells
  - Adapt or develop new biophysical models for new techniques
    - FLASH, mini-beam therapy, VHEE, IRT, NP…..
  - Combine the models to tumoral growth simulations
  - Combine to statistical analysis of clinical data





Borran et al., 2018. Rad. Phys. Chem.

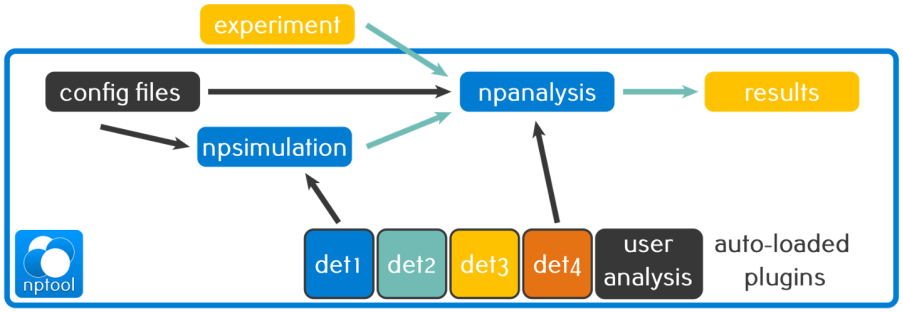
- **A new major release of GATE 10. will be published in about 1 year**
  - Complete refont of C++ classes with Python encapsulation for a more flexible user interface and a better compatibility with all analysis codes written in Python

The nptool project

nptool: key concepts

Key concepts

- A common framework for low energy nuclear physics
- Best use of Root and Geant4
- In use since 2008
- Modular design:
  - Detector and Event Generator as plugins
  - Tool box: tracking, nuclear data, scorer ,…

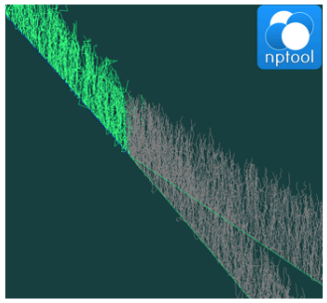


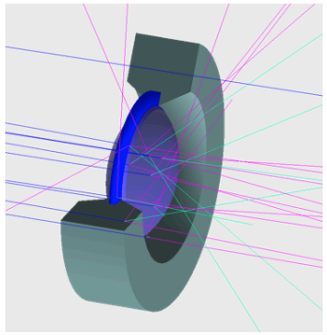
Collaboration

- Framework team: A. Matta, F. Flavigny (LPC Caen), N. de Sereville (IJCLab), V. Alcindor (TU-Darmstadt), P. Morfouace (CEA-DAM), M. Labiche(STFC)
- World wide user base: France, Germany, UK, Spain, Italy, Finland, Norway, Romania, USA, Canada, Japan, India
- Open collaboration: every body is welcome
- Ref. Article : J. Phys. G: Nucl. Part. Phys. 43 045113
- Repo: gitlab.in2p3.fr/np/nptool. Website: nptool.org

The nptool project

nptool: v3 in exploitation





A lot of detectors to choose from (~ 70)

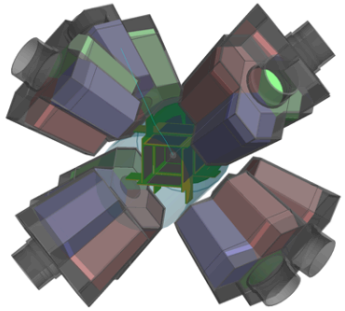
- Silicon (Hira, Share, T-Rex, Grit,…)
- HPGe (Agata, Miniball, Exogam,…)
- Gas (Actar, Minos, Tactics,…)
- Scintillator (Paris, Fatima, Nebula,…)
- Magnetic (ISS, Samurai, Swiper,…)
- Cryo Target w/ deformation

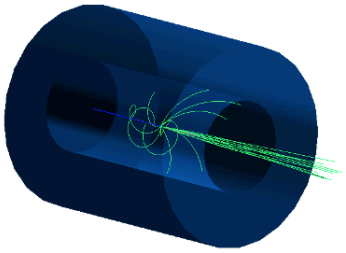
Event generator and physics

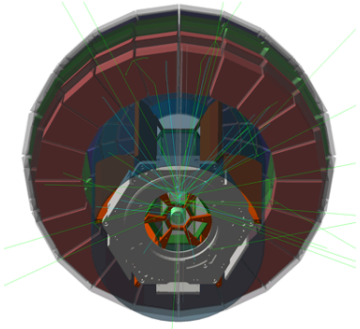
- Direct reaction with CS : transfert, coulex, knock-out
- Nuclear decay : gamma and particle decay, neutron physics, fission,…
- Drift electron simulation for gaseous detector (TPC, IC,…)

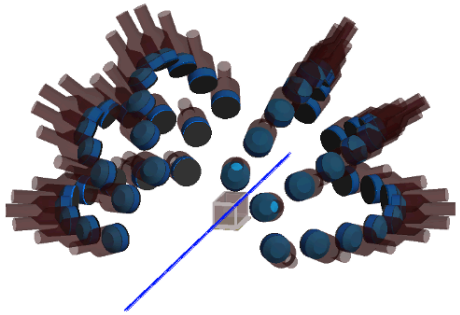
Publications

- Used for about 15 PhD thesis work
- Cited in 24 journal articles









The nptool project

nptool: v4, a pip like experience

Philosophy

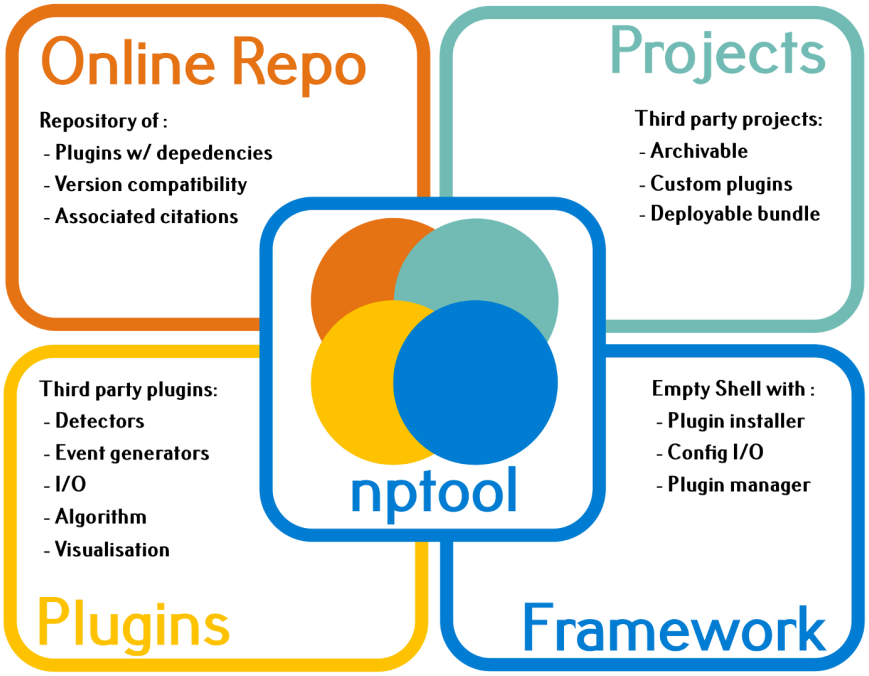
- **Separate plugin and framework**
- **Minimum lightweight installation**
- **Automatic dependencies**

For collaborations

- **Control their own repo. of plugins**
- **Easy CI/CD workflow**
- **Increase visibility with citations utilities**

For end user

- **Plugins on demand**
- **Hassle free installation**
- **Custom projects w/ duplicate plugins**
- **Open science friendly (bundle, archive and containers)**

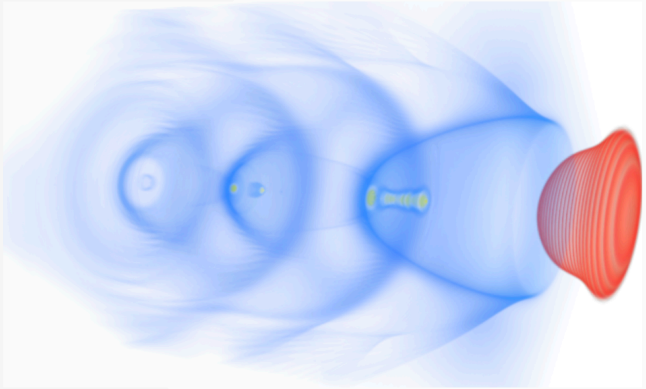


beta version under test /release in 2023

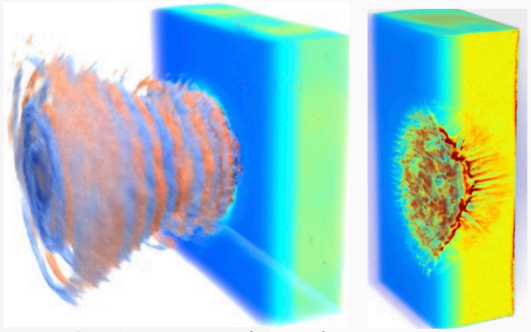
The Smilei project

Smilei is a Particle-In-Cell (PIC) code for the simulation of plasmas

Laser Plasma Interaction

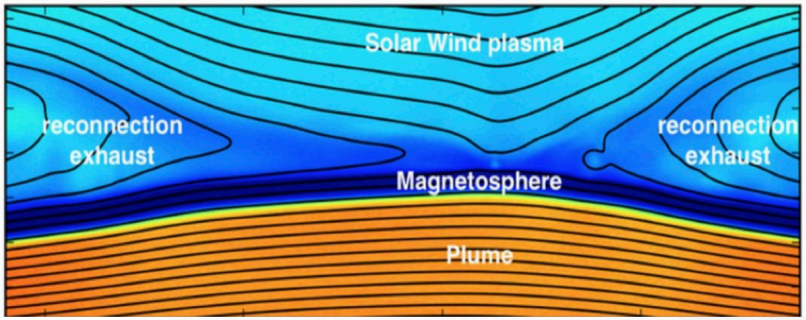


source: Massimo et al. (2020)



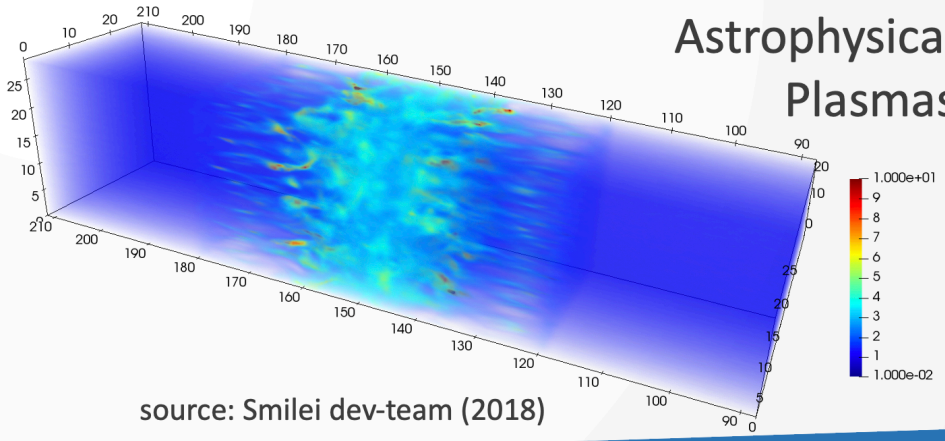
source: Smilei dev-team (2018)

Space Plasmas



source: Dargent et al. (2017)

Astrophysical Plasmas



source: Smilei dev-team (2018)

The Smilei project

Smilei is massively parallel and anchored in the HPC landscape

Integration in the French & European HPC landscapes

GENCI
Le calcul intensif au service de la connaissance

EuroHPC
Joint Undertaking

- Running on all super-computers in France (and many in Europe)
- 10s millions computing hours every year via GENCI & PRACE
- GENCI technological survey
- French Exascale Project

Special/early access to various machines

2015 IDRIS/Turing BlueGene-Q
2016 CINES/Occigen
2018 TGCC/Irene-Joliot-Curie
2019 IDRIS/Jean Zay
2021 RIKEN/Fugaku

The Smilei project

Smilei main contributors: Co-development between physicists & HPC specialists

Core dev-team

Mickael Grech*
Frederic Perez*
Tommaso Vinci*

Arnaud Beck*
Guillaume Bouchard

Mathieu Lobet*
Francesco Massimo*
Res. Engineer**

Computing centers and manufacturers

Physics Laboratories

The code

- 150 000 lines of code
- C++ 85% / Python 15%
- 300 man.months in dev. only
- 10's MCPUhours every year
- CeCILL-B licence / Github

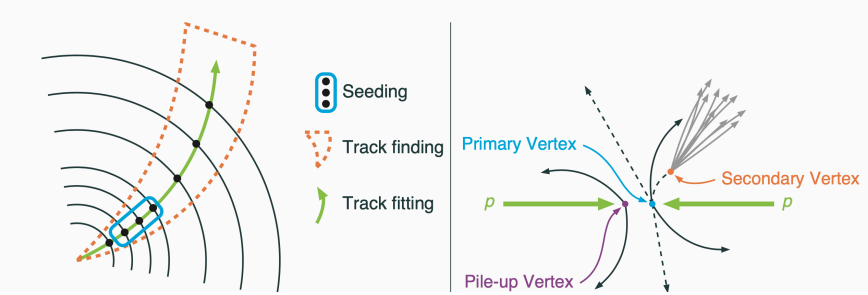
*permanent staff **Res. Engineer position to be opened (CNRS DDOR, w.s.f. INP, INSU, IN2P3)

Data Processing and analysis

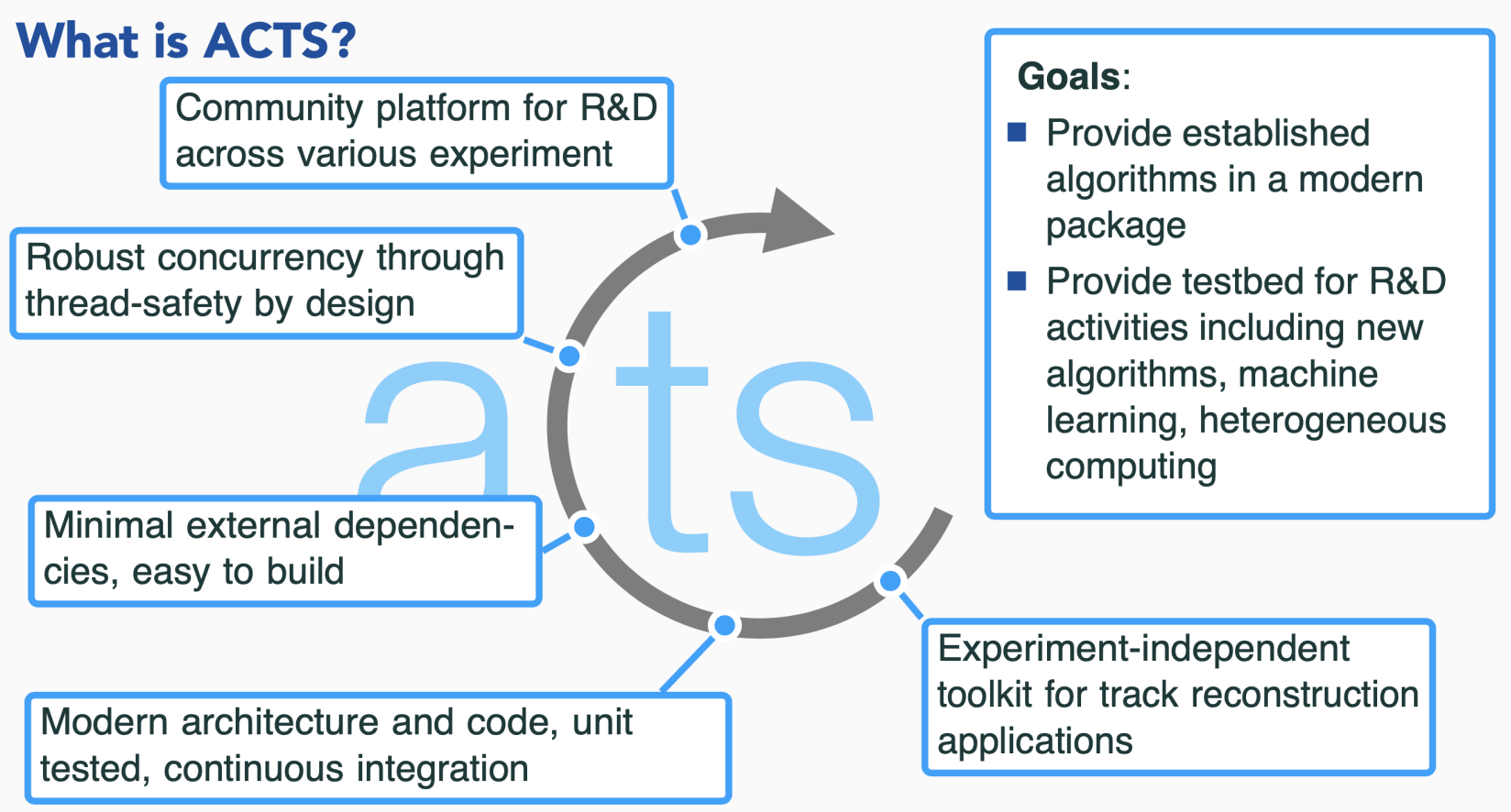
- **Toward common software solutions** for multiple experiments/ communities
- **ACTS** (A Common Tracking Software) (HEP community)
  - **Experiment-independent** toolkit for track reconstruction
- **Gammapy** (astroparticle community)
  - A python package for high-level γ-ray astronomy based on **common data formats**
- Similar effort in the nuclear physics domain, where traditionally each group was developing its own software
- **AGATA software**
  - On-line processing of data produced with the AGATA detector
- **KaliVeda**
  - Data processing and analysis for the INDRA and FAZIA detectors
- **nptool**
  - Data processing (and simulation) for low energy experiments

The ACTS project

- Scientific challenges
  - The reconstruction of charged particle trajectories is one of the most complex and CPU consuming parts of event processing in HEP experiments
  - Even more challenging with the increased number of simultaneous collisions at HL-LHC and Future Circular Collider
- A Common Tracking Software (ACTS)
  - Experiment-independent toolkit for track reconstruction
  - Originally launched by the ATLAS tracking group in the 2010s
  - Today several contributors from CERN, LBNL, CNRS/IN2P3, University of Geneva, Eotvos Lorand University in Budapest and Max-Planck Institute for Physics

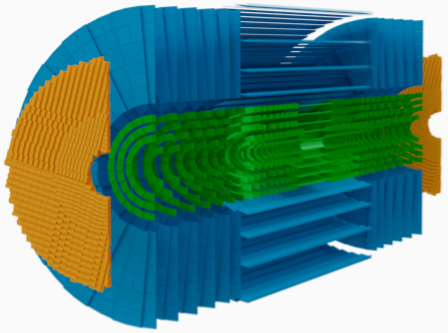


The ACTS project

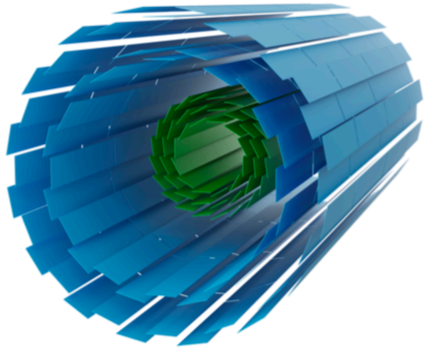


The ACTS project

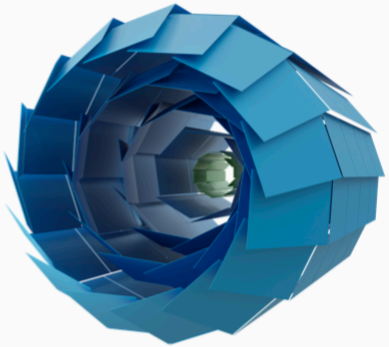
Evaluation and/or deployment by multiple experiments



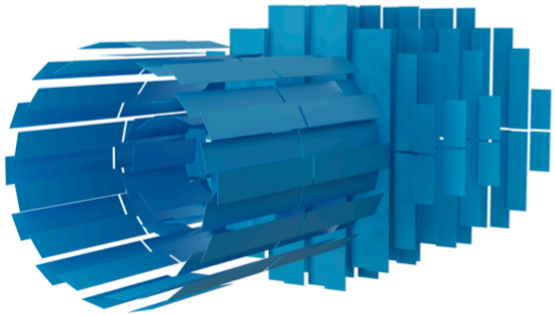
ATLAS Inner Tracker



sPHENIX

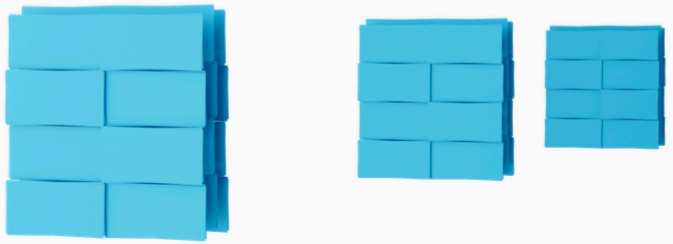


Belle II



Panda

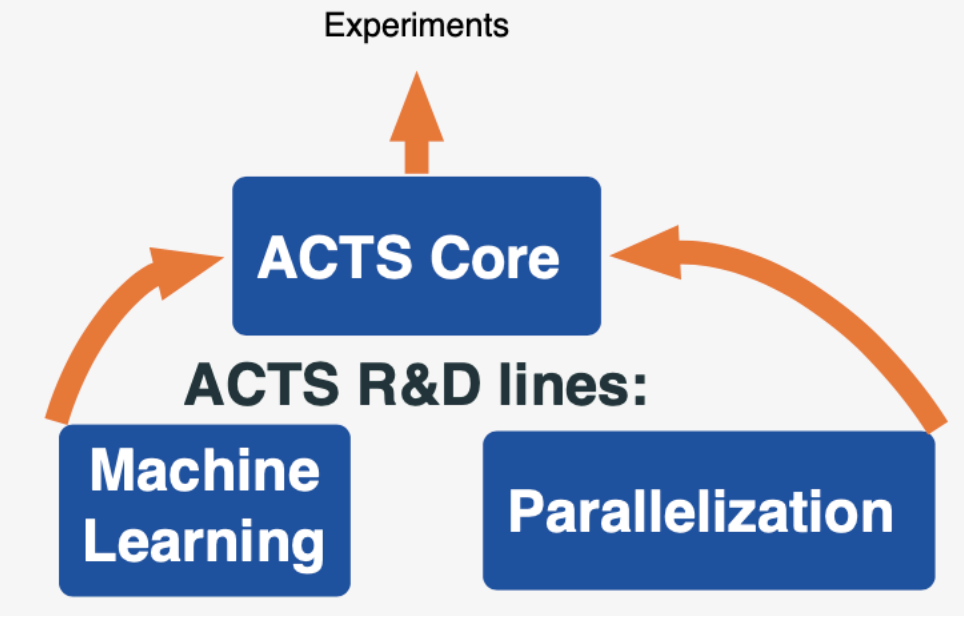
+ ALICE,
EIC



FASER

The ACTS project

- Mature project, ready for a progressive adoption within ATLAS
  - It will allow for an extensive validation
  - It will encourage its adoption by other experiments
- R&D activities



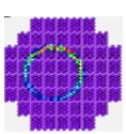
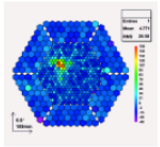
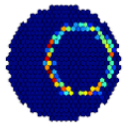
The ACTS project

- ACTS core development team ~ 10 persons, mainly at CERN and US universities
- IN2P3 contribution < 10% (1.8 FTE) in the past years, but now increasing
  - **Recent recruitment of 1 post-doc at IJCLab and 1 post-doc at LAPP**
- GPU R&D at IN2P3
  - Development of tracking algorithms suitable to run on GPU
  - The goal is to have a full reco chain demonstrator on GPU by the end of 2022
  - **Evaluation of SYCL** (GPU programming model w/o Nvidia lock-in) **(IJCLab)**
- Machine Learning R&D at IN2P3
  - **IJCLab** involved since long (**TrackML challenge**), more recently also LAPP and L2IT started to actively contributing
  - **AIDAinnova** : auto-tuning of tracking algorithm parameters, involves work on Python bindings **(CERN, IJCLab)**
  - **ATRAPP ANR** : Spatial hashing, integration of detector conditions, anomaly detection, … **(LAPP, IJCLab)**
  - Development of **Graph Neural Networks** tracking algorithms **(L2IT)**

Gammapy
A Python package for gamma-ray astronomy

Proprietary formats and tools

- All instruments have their own proprietary formats and tools
  - usually based on the open software ROOT from CERN
- Common joint analyses are impossible

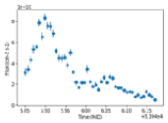
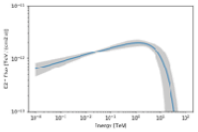
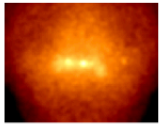




Raw data

H.E.S.S.

MAGIC

VERITAS

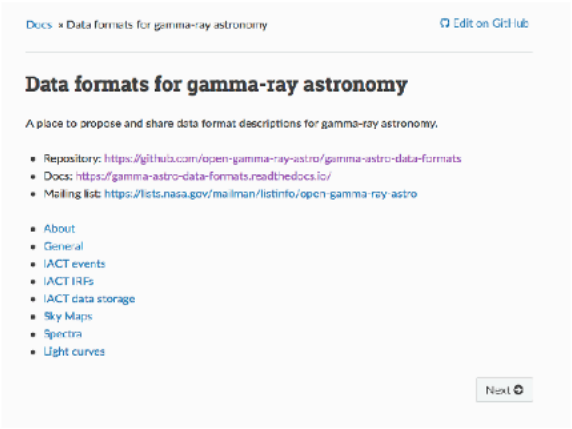
High level science products

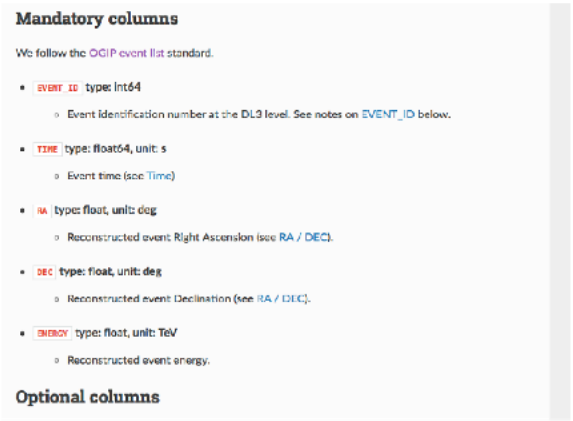
Interoperability & reusability require common open *data formats* and common open *tools*

Gammapy

Towards common data formats

- A community initiative to provide open data formats for VHE astronomy
  - g.a.d.f. (gamma-ray astro data formats) :a prototype format
  - VHE common formats initiative with people representing
    - pointing Cherenkov telescopes (e.g. CTA, Veritas, MAGIC etc)
    - drifting telescopes (e.g. HAWC, SWGO and Km3Net, IceCube)
    - Fermi-LAT





The data flow

Separating instrument specific data treatment from common use cases and methods

Reconstruction pipeline (internal) → Science Tools (general users)

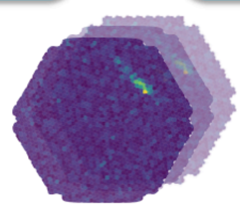
DL 0-1 — *raw - calibrated*

DL 2 — *reconstructed*

DL 3 — *filtered γ-like events*

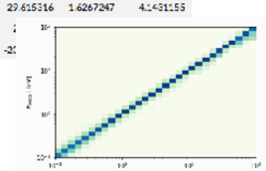
DL 4 — *science*

DL 5 — *high-level*

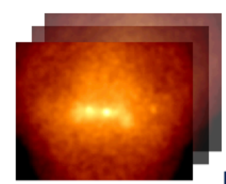


camera data

ENERGY	RA	DEC	L	B
MeV	deg	deg	deg	deg
float32	float32	float32	float32	float32
12186.642	260.45935	-33.553337	353.36273	1.7538676
25496.598	261.37506	-34.395004	353.09607	0.6520652
15621.498	259.56973	-33.409416	353.05673	2.4450684
12816.32	273.95883	-25.940391	6.45856	-4.0548879
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	-26.224436	[illegible]	[illegible]
13960.802	271.44742	29.615316	1.6267247	4.1431155
10477.372	266.3981			
13030.88	271.70128			



γ-like event lists
IRFs



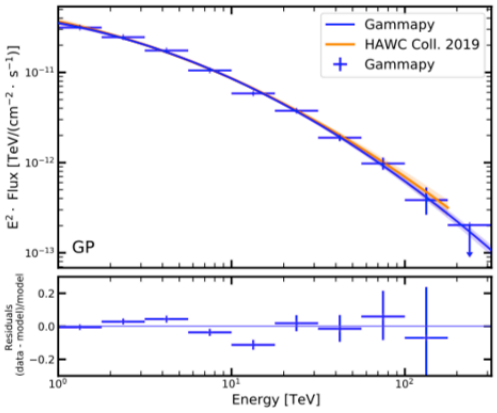
maps,
spectra,
light curves

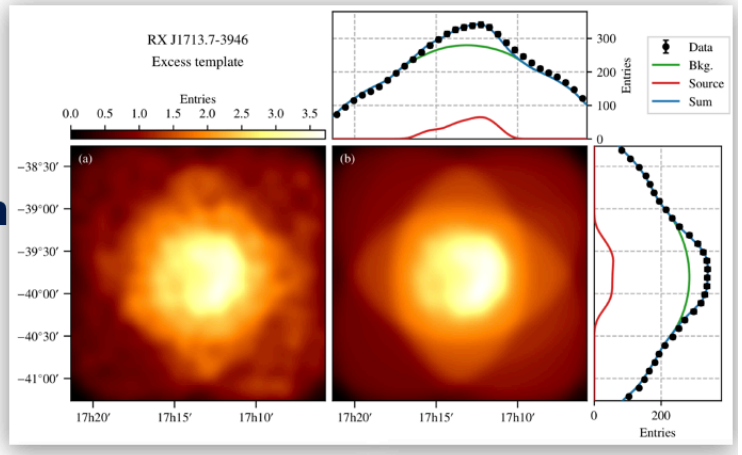
Gammapy

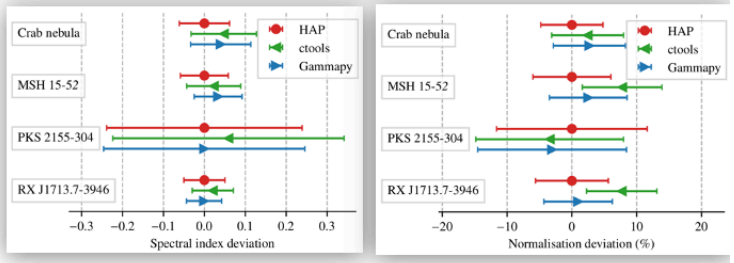
Science validation & maturity

Science usage validated on HESS DL3 test data release

- **Selected as science tool library by CTAO**
- **Now regularly used for science publications in HESS collaboration**
- **Prototype analyses with HAWC**







Olivera-Nieto et al (2021)

Mohrmann et al. (2019)

Gammapy

Gammapy project organisation

Coordination committee

Project managers
Bruno Khélifi at APC & ECAP

Lead developers
Régis Terrier at APC & MPI-K

Developers
About 10 regular contributors
More than 80 contributors in total

More formal structure of the project introduced to ensure development planning and improve interactions with experiments/observatories

About 30 FTE in total and 12.3 FTE at IN2P3 from 2015 to 2022
2 permanent staff at APC in the roles of Project Manager (B. Khélifi) and Lead developer (R. Terrier)

Data processing software for AGATA

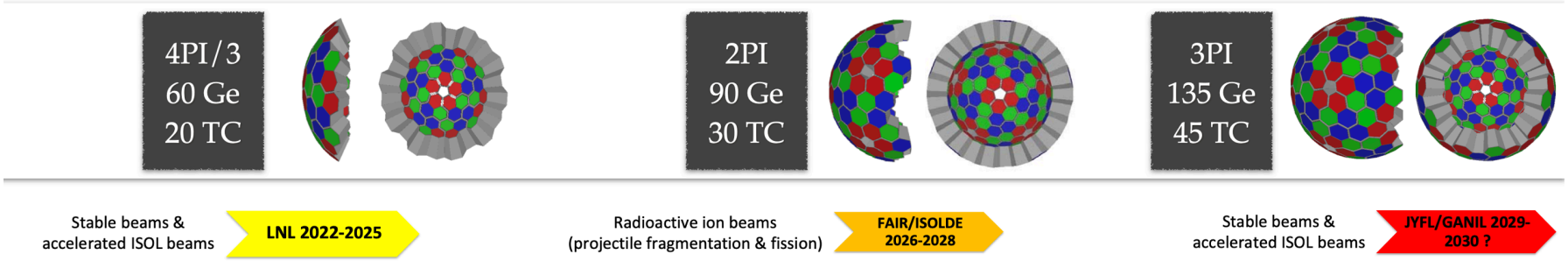
AGATA
Advanced Gamma-ray Tracking Array

Ultimate goal: tracking of gamma-rays in a Germanium 4Pi ball

AGATA is a nomad array built by an European collaboration (~12 countries)

MOU
Phase 1
2010-22

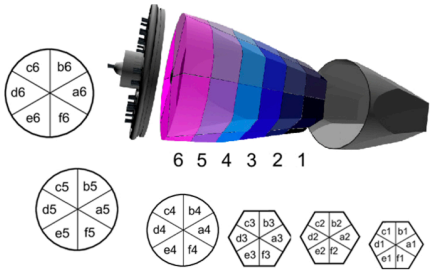
MOU - Phase 2 - 2022-30



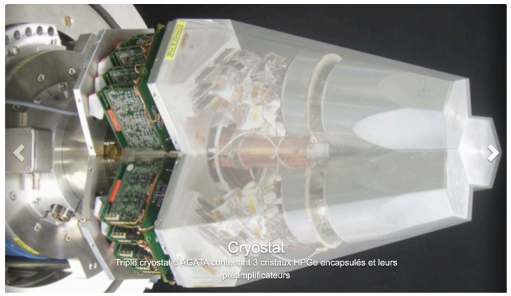
Data processing software for AGATA

AGATA : INGREDIENTS

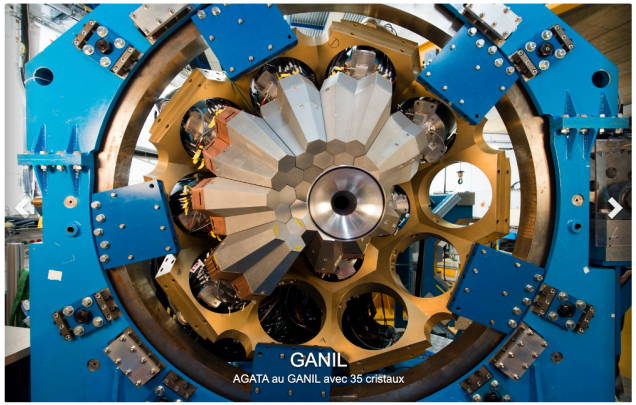
2 key algorithms PSA (Pulse Shape Analysis) and Tracking



High Purity Germanium crystal
36 segments + 1 core digitized signals



Cluster composed of 3 capsules



Assembly of clusters around the target

Global level data pipeline

N crystals

Event
hits of all crystals

Builder

ancillaries

Merger

Charged particles
Neutrons
Recoils etc …

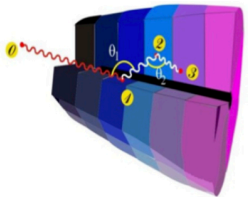
γ Tracking

Tracked gamma-rays

Local level data pipeline

37 signals

PSA

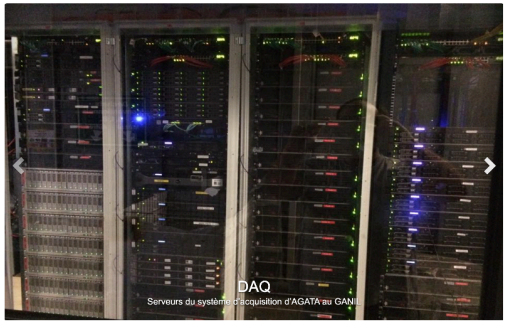


List of hits for one crystal

Data processing software for AGATA

AGATA : Computing (+R&D) @ IN2P3

The 2 key algorithms are continuously improved
Same for the harware and software infrastructure to run them



In charge of the Online Computing infrastructure

Services and computing nodes : ~ 70 servers
CEPH storage ~ 500 Tb, ~ 130 Tb (RAID mode)

Maintenance / upgrades / adaptation

Provide the online workflow management

DCOD written in ADA, developed @ IJCLab
Topology manager

Maintenance / upgrades / adaptation / R&D

IN2P3

Involved at many levels in the data pipelines

Code tracking dev. @ IJCLab
Online monitoring dev. @ IP2I
Production of root trees dev. @ IP2I
…

Maintenance / upgrades / R&D

IN2P3 involved since 2009 in AGATA

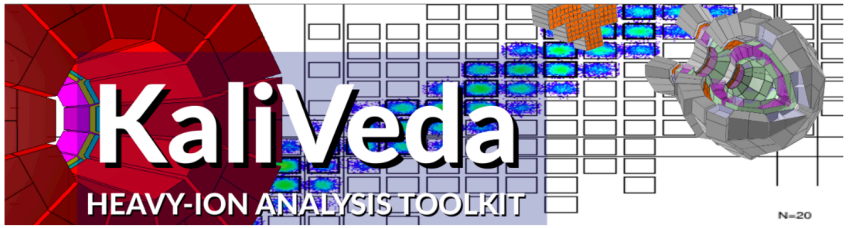
IN2P3 effort to software activitiy is ~ 5 FTE

Some key words on the IN2P3 activities

C++ / ADA / modern cmake / git / continuous integration / docker
code profiling / multithread / simulations / grid for storage …

R&D : Machine Learning (PSA/Tracking) / GPU / REDIS /
HPC / Time series databases …

KaliVeda Heavy-Ion Analysis Toolkit



C++ toolkit based on ROOT for analysis & simulation of Fermi energy heavy-ion collisions

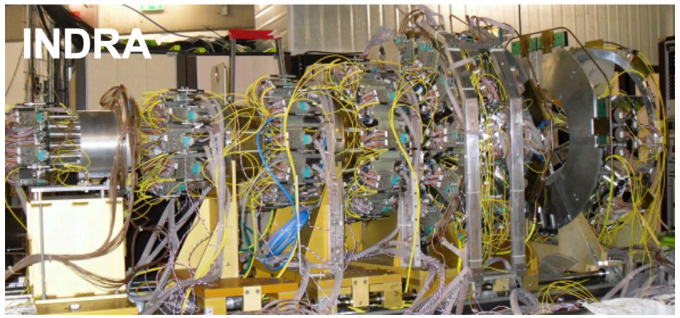
Main developers/maintainers:
John Frankland (CRHC GANIL Caen)
Diego Gruyer (CRCN LPC Caen)
Eric Bonnet (CRCN SUBATECH Nantes)

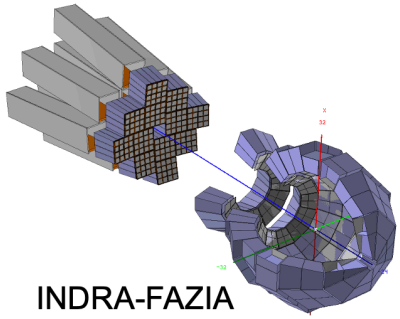
. Developed since 2002 to provide a unified environment for INDRA data reduction & analysis

- Since 2014, also used for the FAZIA array (and the INDRA-FAZIA coupling since 2019)
- Basis for all slow control GUI used during INDRA & FAZIA experiments

. Main features:

- Simulation & calibration of charged particle (ions) energy losses in detectors of different types
- Many tools for Z & A identification of ions using either ΔE-E or PSD techniques
- Single environment for analysis of all INDRA data since 1993 at CC-IN2P3 (batch) or on multi-core PC (PROOFLite)





INDRA-FAZIA experiment
E818 geometry (2022)

Workload, data and metadata management

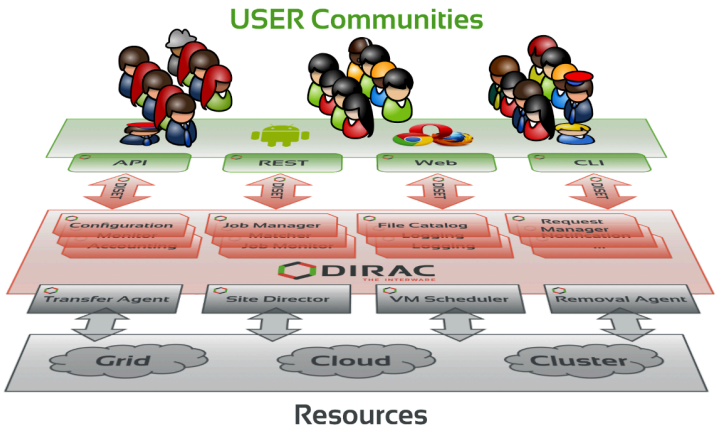
- The usage of large computing infrastructures and the production of large amount of complex scientific data requires **adavanced Management softwares**
- Solutions developed within LHC experiments, today adopted by several communities in HEP and beyond
- **DIRAC**
  - Workload Management (i.e. of computing tasks) in distributed and heterogenous computing environments (grids, clusters, …)
- **AMI**
  - A generic ecosystem for the handling of scientific metadata

The DIRAC project

DIRAC
THE INTERWARE

What's DIRAC?

- A software framework for distributed computing
- A **complete** solution to one (or more) user community
- Builds a layer between users and resources



- Started as an LHCb project, experiment-agnostic in 2009
- Developed by communities, for communities
  - Open source (GPL3+), GitHub hosted
  - Python 3 (python 2.7 kept for current production release)
  - Publicly documented, active assistance forum, yearly users workshops, open developers meetings and hackathons
- The DIRAC consortium as representing body

The DIRAC project

DIRAC
THE INTERWARE

Installations and communities

A *framework* shared by multiple experiments/projects, both inside HEP, astronomy, and life science

Experiment agnostic
Extensible
Flexible

The DIRAC project

IN2P3 Master Project

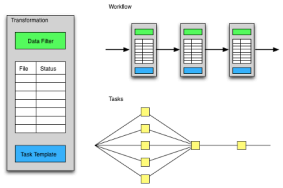
- The project started in 2017
  - Scientific Coordinator: A.Tsaregorodtsev, **CPPM**
  - Technical Coordinator: J.Bregeon, **LPSC**
- Participants
  - IN2P3: **CPPM, LUPM, LPSC, IPHC, CC/IN2P3**
    - **12 research engineers for 2.3 FTE**
  - CNRS/INSERM/INSA/U.Lyon/U.St.Etienne: **CREATIS**
- Goals
  - Federate the French actors around DIRAC
  - R&D for the needs of new scientific communities and technology advances

The DIRAC project

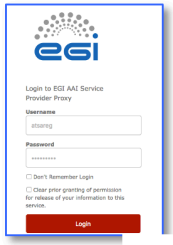
DIRAC
THE INTERWARE

Selected developments

- Production System for high level workflow management of large scientific communities
- Integration of various computing resources: cloud, HPC
- Support for OAuth2/OIDC based AAI systems (EGI Check-In, WLCG IAM)
- Application of Go language for distributed computing systems



openstack



slurm
workload manager

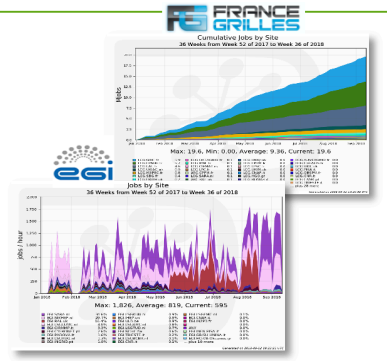
GO

The DIRAC project

DIRAC
THE INTERWARE

Collaboration

- EGI Workload Manager Service
  - Hosted at CC/IN2P3
  - ~10M jobs per year
  - ~40 VOs, 700 registered users
- DIRAC user's support
  - Support for DIRAC services: IHEP, JINR, …
  - CTA, HESS, biomed, Eiscat 3D, WeNMR …
- DIRAC service in the ESCAPE Project catalogue
  - Concordia for running containerized Corsika applications
- Coordination of the DIRAC Consortium
  - Membres: CNRS, CERN, IHEP, KEK, Imperial College, University of Montpellier
  - Managing software releases, web site
  - DIRAC Users' workshops



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

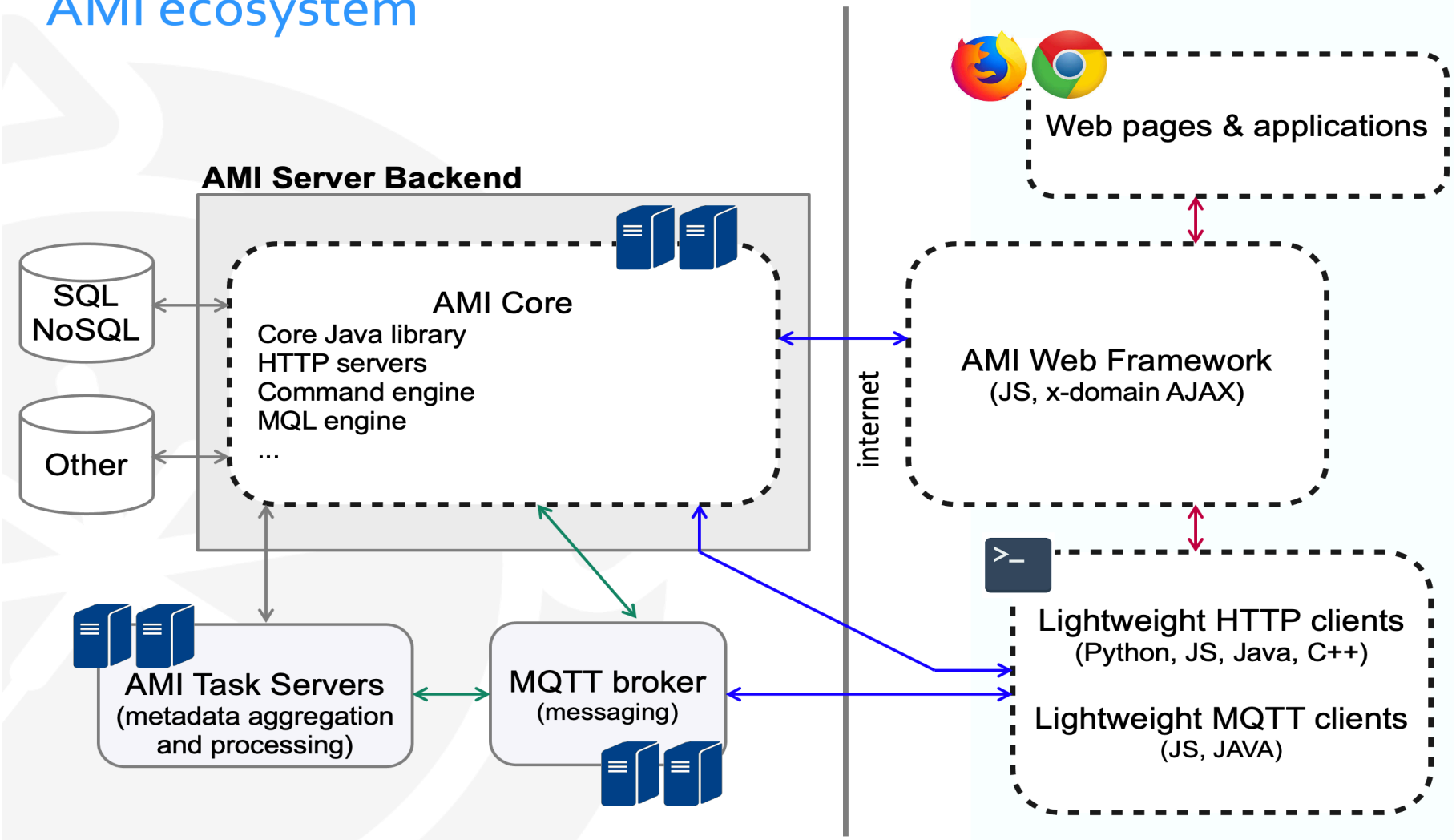
The AMI project

What is AMI?

- **AMI (ATLAS Metadata Interface) is a generic ecosystem for scientific metadata**
  - Complete solution from end-user applications down to DataBases including
    - Primitives for metadata extraction and processing
    - High level tools for selecting data by metadata criteria
    - Users base management…. and more
- AMI originally designed for ATLAS
  - Manage metadata for all ATLAS datasets and ATLAS software configurations **(~500M files, 260Gb per year, ~5K users)**
  - **Recent major re-write after ~20 years**
- Latest version entirely generic
  - Connect to any DB, deployable with docker
  - Used in other experiments : Nika2,… ?
  - **Designed for : Scalability, evolutivity and maintainability**

The AMI project

AMI ecosystem



The AMI project

Summary on AMI

- AMI (ATLAS Metadata Interface) is a generic ecosystem for scientific metadata
  - Complete solution from end-user applications down to DataBases

- **Actively developed at LPSC**
  - 3 FTE: J. Fulachier, F. Lambert, J. Odier (engineers) M. Jaume (Student)
  - Resources just enough for development and maintenance

- **Plans**

- Continue the development effort to cope with the needs of ATLAS for the Run3 and HL-LHC
  - Welcoming new users
  - Attract new developers

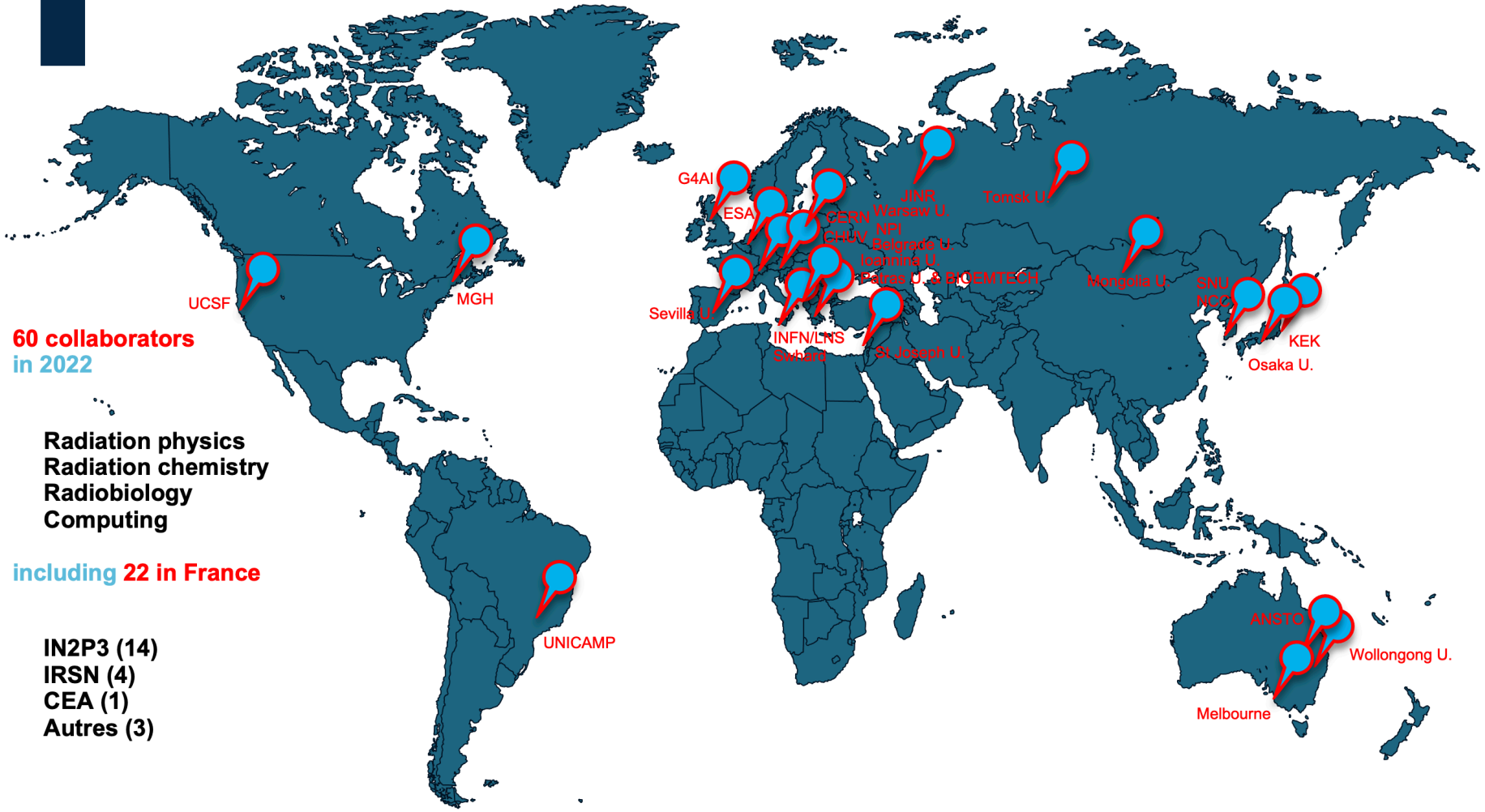
Conclusions

- Strong involvement of IN2P3 staff in several key projects in collaboration with our international partners
- Management responsibility in several projects
- Good synergies among projects around Geant4
- People very active also in dissemination and training actions
- Very large and worldwide-spread users communities
- IN2P3 staff also involved in several R&D activities
- R&D topics are common to several projects : machine learning, GPU, exploring new hardware, …
- Importance of the recruitment of permanent staff to effectively contribute to complex projects and to ensure the long-term development
- Importance of collaborations with “computing experts” (computer scientists, computing centers, manufactures, …)

Backup

The Geant4-DNA project

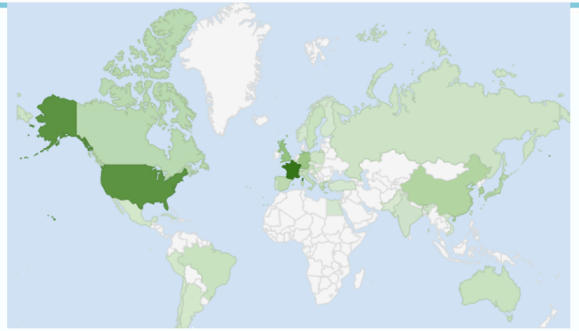
An international collaboration



- **60 collaborators in 2022**
  - Radiation physics
  - Radiation chemistry
  - Radiobiology
  - Computing
- **including 22 in France**
  - IN2P3 (14)
  - IRSN (4)
  - CEA (1)
  - Autres (3)

The GATE project

A large community of users



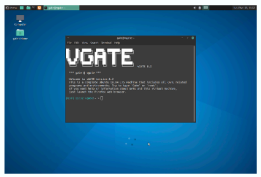
Around 2000 registered users

- Large communities in France and USA
- Increasing community: Canada, UK, Australia, Germany, China, Japan

Open source and open access platform available on Github

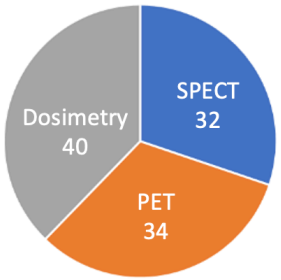
The source code: https://github.com/OpenGATE/Gate
The examples: https://github.com/OpenGATE/GateContrib
The tools for analysis: https://github.com/OpenGATE/gatetools

GATE version 9.2
1 release/year



Trainings & Workshops

- 1 workshop / conference of interest: IEEE NSS-MIC, AAPM, MCMA, PTCOG…
- Trainings for beginners: 1/year and @ companies
- Advanced trainings: 1/year (Python data analysis…)



Papers – Period: 2015-Now (PubMed search)

The GATE project

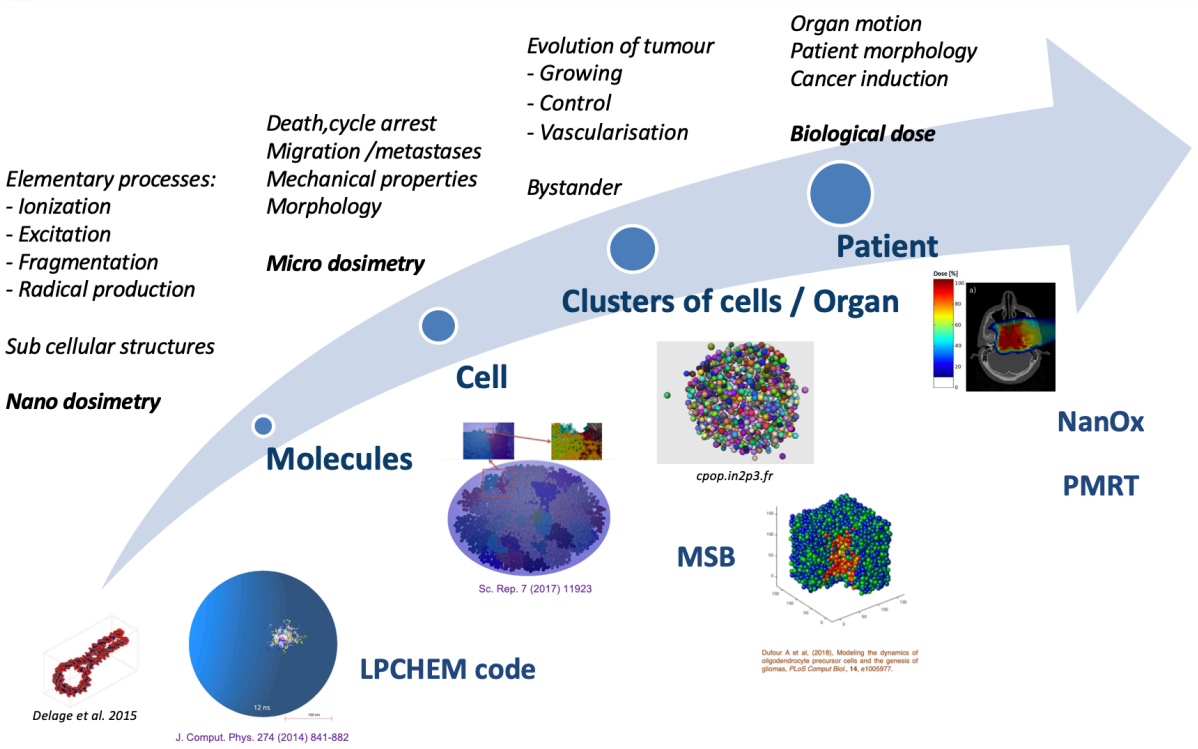
Multi-scale simulations

GEANT4-DNA

The **unique** open source and open access simulation toolkit for micro/nano dosimetry and radiation biology

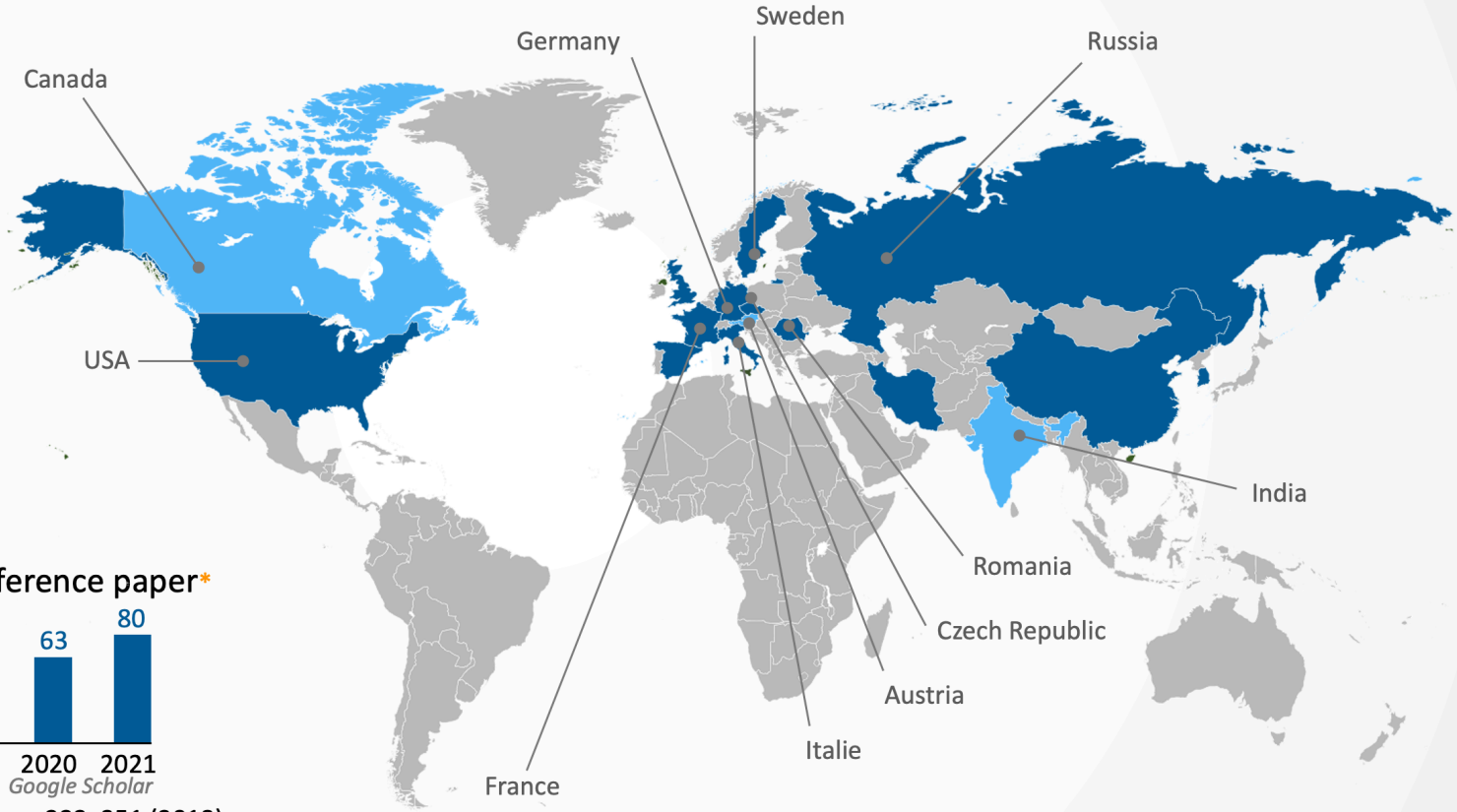
- **Long term development** fully included in Geant4 releases
- International collaboration composed of 42 collaborators
- **Coordinated by IN2P3/CNRS** since 2008
- Funded by regular support from institutions and international calls
- Fruitful involvement in international conferences & tutorials
  - Geant4 International User Conference at the Physics-Medicine-Biology frontier » series of conferences initiated by IN2P3 in 2005
  - Annual international tutorials (17)
- High rank and highly cited publications (104 since 2007)

DEVELOPMENT ACCESSIBLE TO OTHER TOOLKITS, PARTICULARLY TO GATE

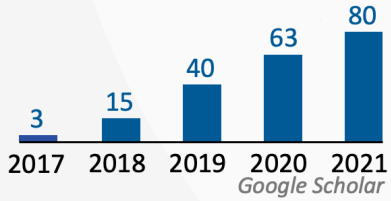


The Smilei project

Smilei's user community is international & steadily growing



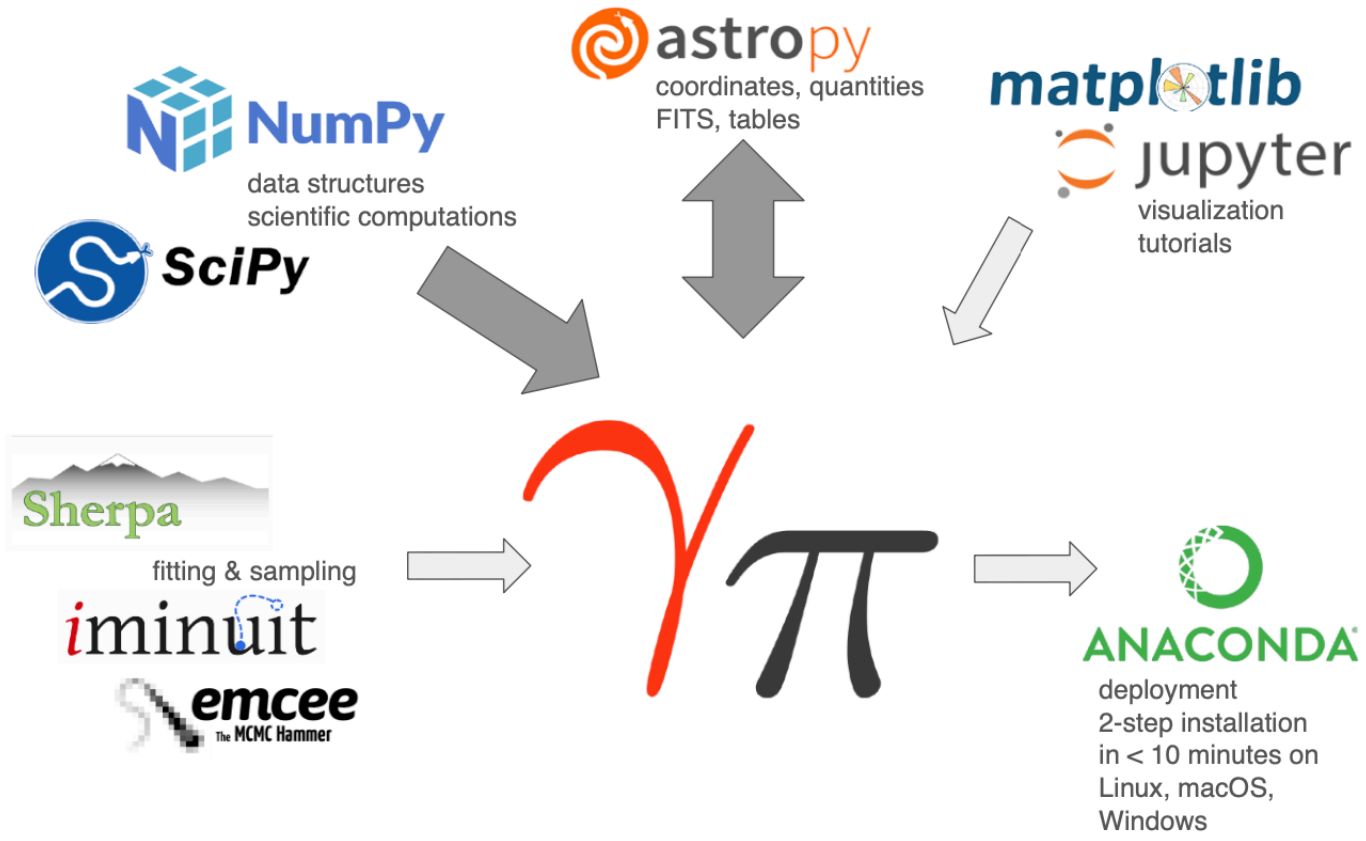
200+ citations for Smilei reference paper*



*Dérouillat et al., Comp. Phys. Comm. 222, 351 (2018)

Gammapy

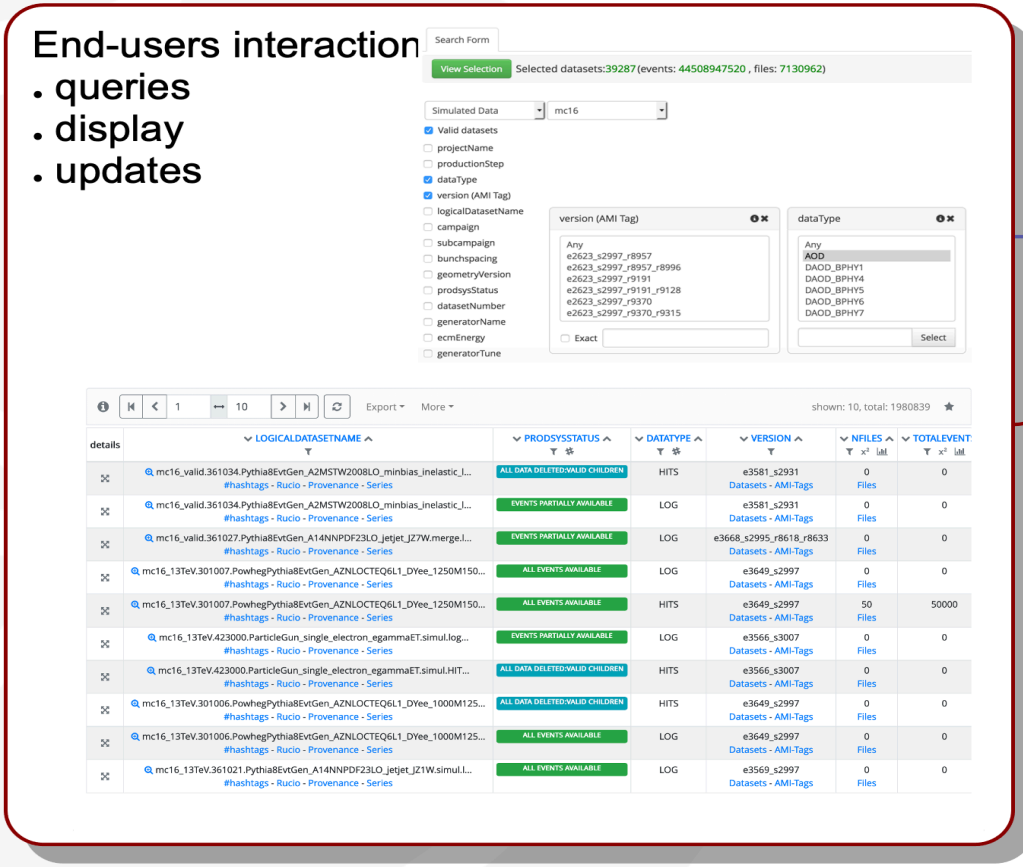
Gammapy in the Python ecosystem



The AMI project

AMI ecosystem

End-users interaction
- queries
- display
- updates



internet

Web pages & applications

AMI Web Framework
(JS, x-domain AJAX)

The AMI project

Major AMI feature : MQL

Metadata Query Language

- Query language dedicated to metadata
  - Simpler than SQL
  - Independent of underlying DB organisation
- Unique implementation in AMI
  - AMI has **reflexion** capability (automatic discovery of existing BD structures)
  - Internal translation from MQL → SQL

```
SELECT * WHERE (`AMISTATUS` = 'VALID')
               AND
               [`DATASET_KEYWORDS`.`KEYWORD` = 'stau']
               AND
               [`KEYWORD` = 'stop']
```

MQL to SQL

```
SELECT * FROM `ATLAS_AMI_MC16_02`.`DATASET`
WHERE
  (
    `ATLAS_AMI_MC16_02`.`DATASET`.`AMISTATUS` = 'VALID'
  )
  AND (
    `ATLAS_AMI_MC16_02`.`DATASET`.`IDENTIFIER` IN (
      SELECT
        `ATLAS_AMI_MC16_02`.`DATASET`.`IDENTIFIER`
      FROM
        `ATLAS_AMI_MC16_02`.`DATASET_KEYWORDS`,
        `ATLAS_AMI_MC16_02`.`DATASET`
      WHERE
        (
          `ATLAS_AMI_MC16_02`.`DATASET_KEYWORDS`.`KEYWORD` = 'stau'
        )
        AND `ATLAS_AMI_MC16_02`.`DATASET_KEYWORDS`.`DATASETFK` = `ATLAS_AMI_MC16_02`.`DATASET`.`IDENTIFIER`
    )
  )
  AND (
    `ATLAS_AMI_MC16_02`.`DATASET`.`IDENTIFIER` IN (
      SELECT
        `ATLAS_AMI_MC16_02`.`DATASET`.`IDENTIFIER`
      FROM
        `ATLAS_AMI_MC16_02`.`DATASET_KEYWORDS`,
        `ATLAS_AMI_MC16_02`.`DATASET`
      WHERE
        (
          `ATLAS_AMI_MC16_02`.`DATASET_KEYWORDS`.`KEYWORD` = 'stop'
        )
        AND `ATLAS_AMI_MC16_02`.`DATASET_KEYWORDS`.`DATASETFK` = `ATLAS_AMI_MC16_02`.`DATASET`.`IDENTIFIER`
    )
  )
```