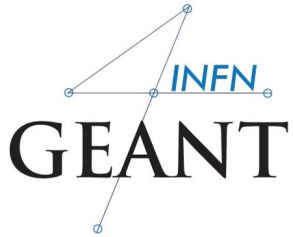
GEANT4, A LONG JOURNEY TO FUTURE

L. Pandola

Laboratori Nazionali del Sud



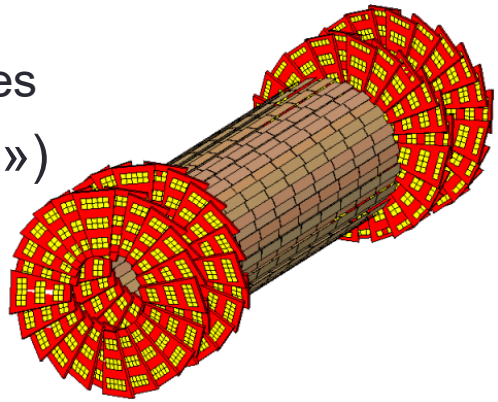
Material and input by G. Bartolini, B. Caccia, G.A.P. Cirrone, F. Farokhi, S. Fattori, C. Mancini Terracciano, G. Milluzzo, G. Paternò, G. Petringa, I. Postuma, S. Pozzi, F. Romano, A. Sciuto, A. Sytov

Computing@CSN5: applications and innovations at INFN
Bari, October 14th-16th 2024

INTRO & HISTORY

Introduction

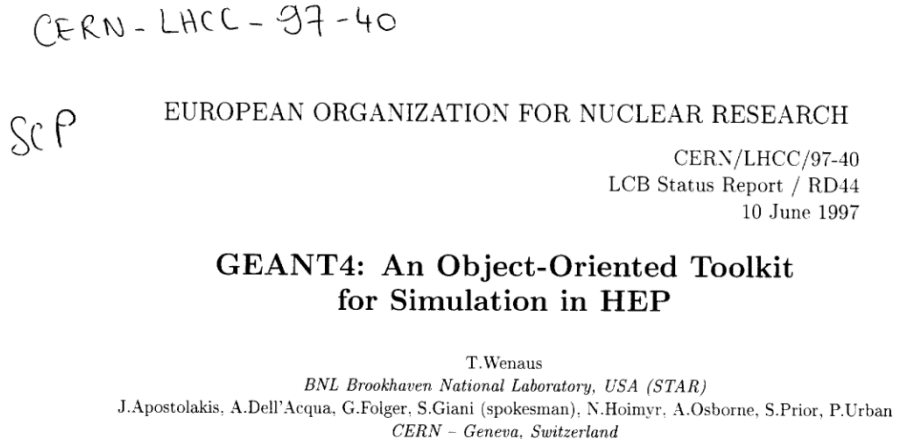
- **Monte Carlo simulation** of the interaction of **ionizing radiation** with matter key ingredient for all particle and nuclear physics experiments
  - … and astroparticle, space, medical, applied physics, …
- **Highly transversal need** within all **INFN communities**
- Used both for the design/optimization of experiments and for the data analysis phase
- **Must** feature:
  - Reliable physics models → key!
    - At least in a specific energy range and for a set of particles
  - Capability to handle complex geometries («navigation»)
  - Computational efficiency («be fast»)



A little bit of history… R&D to Geant4

- A new toolkit for the **simulation** of the interaction of **particles** with **matter,** meant to be the successor of the FORTRAN-based Geant3
  - CERN product, widely used in the ‘90
- Start as **R&D project** (RD44) at **CERN** (1994-1998)
  - Definition of the basic strategy and design
  - Initiated for HEP, but with a **broader perspective** since the beginning
  - Geant4.0.0 Production Release in December 1998

- Main aspects/novelties:
  - Written in **C++ language**
    - Takes advantage from the Object Oriented software technology
    - Easy to extend
  - **Open source**



CERN-LHCC-97-40

SCP

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

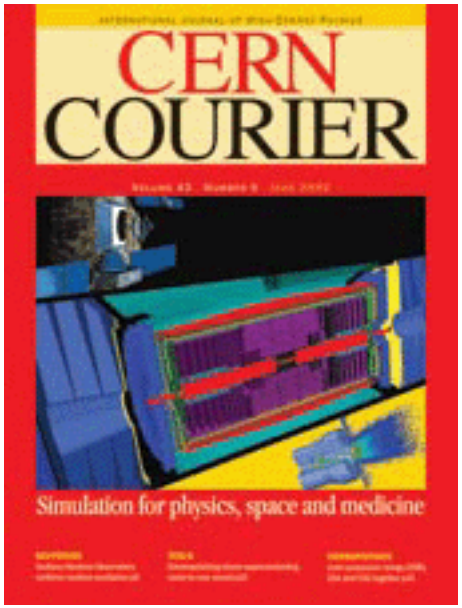
CERN/LHCC/97-40
LCB Status Report / RD44
10 June 1997

GEANT4: An Object-Oriented Toolkit for Simulation in HEP

T.Wenaus
BNL Brookhaven National Laboratory, USA (STAR)
J.Apostolakis, A.Dell'Acqua, G.Folger, S.Giani (spokesman), N.Hoimyr, A.Osborne, S.Prior, P.Urban
CERN – Geneva, Switzerland

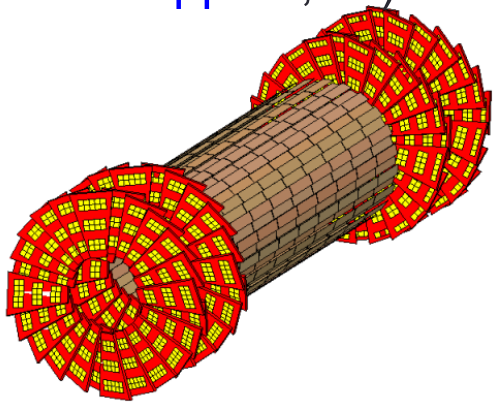
The Geant4 Collaboration!

- **International Geant4 Collaboration born in 1998**
  - Approximately 100 members, from Europe, America and Asia
  - Last week, 29th Collaboration Meeting (hosted in Catania)
- Regulated by its own **MoU**, with spokesman and other boards
  - Current spokesman: Alberto Ribon (CERN), 2-year terms
- **INFN** in the game since the very beginning, with a leading role
- Effective organization in **working groups**
- **Takes care** of software production and management
  - Regularly, two releases per year since >20 years (+ patches)
  - Examples released with the kernel → many domains, including applied physics
- Last version: **Geant4 11.2.p02** (Jun 21st, 2024)



Story of a success…

- Geant4 immediately **recognized** and **adopted** in many different domains
  - All «big four» at LHC, but also many experiments/projects
  - Significant use in **medical physics** (Geant4-DNA, several wrappers, …)
- Three papers, highly cited
  - S. Agostinelli et al., NIM A **506** (2003) 250 → 17.5k
  - J. Allison et al., IEEE TNS **53** (2006) 270 → 4.7k
  - J. Allison et al., NIM A **835** (2016) 186 → 2.3k
  - Growing at *>1300 citations/yr*
- The main Geant4 paper is the 2nd most cited paper in INSPIRES



The Large N limit of superconformal field theories and supergravity #1

Juan Martin Maldacena (Harvard U.) (Nov, 1997)

Published in: *Int.J.Theor.Phys.* 38 (1999) 1113-1133 (reprint), *Adv.Theor.Math.Phys.* 2 (1998) 231-252 • e-Print: hep-th/9711200 [hep-th]

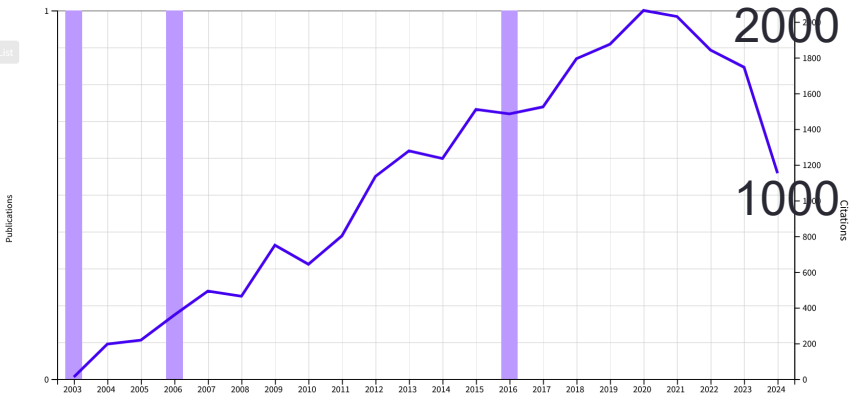
pdf DOI cite claim reference search 20,046 citations

GEANT4--a simulation toolkit #2

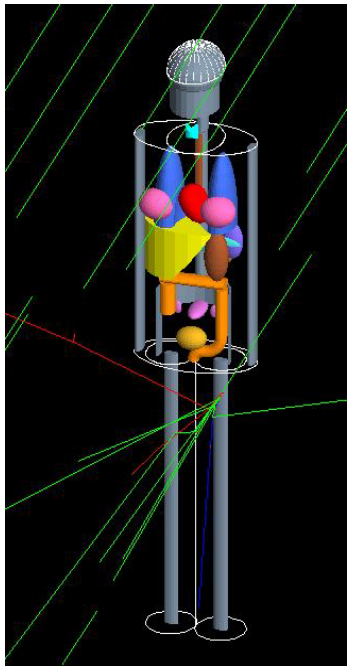
GEANT4 Collaboration • S. Agostinelli (Genoa U.) et al. (Aug, 2002)

Published in: *Nucl.Instrum.Meth.A* 506 (2003) 250-303

pdf links DOI cite claim reference search 19,157 citations

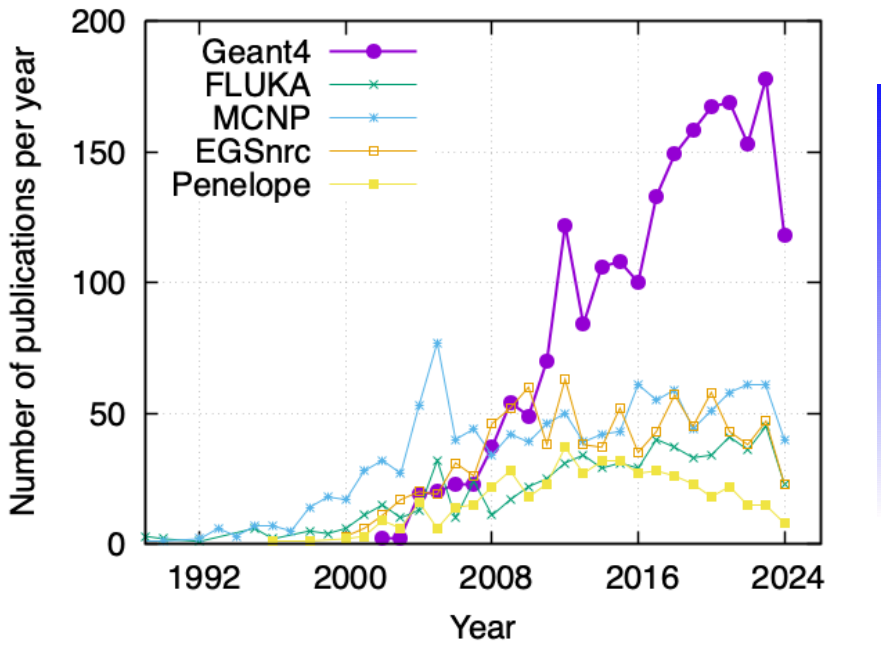


… in many different fields



- Open source + general purpose + flexible for extensions → rapid diffusion to *different domains*
  - Underground/lowenergy, medical, space, nuclear, …
- Other important **drivers**:
  - Active communities represented in the Collaboration
  - Availability of (maintained) examples

- **Highly transversal product**: of interest for most experiments accross all CNSs of INFN
  - Users in applied physics
- **Technology transfer** → use in non-academic application
  - Contribution from INFN

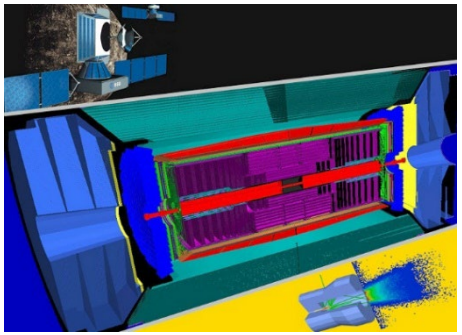


Talk by G. Bartolini

The Geant4 Collaboration

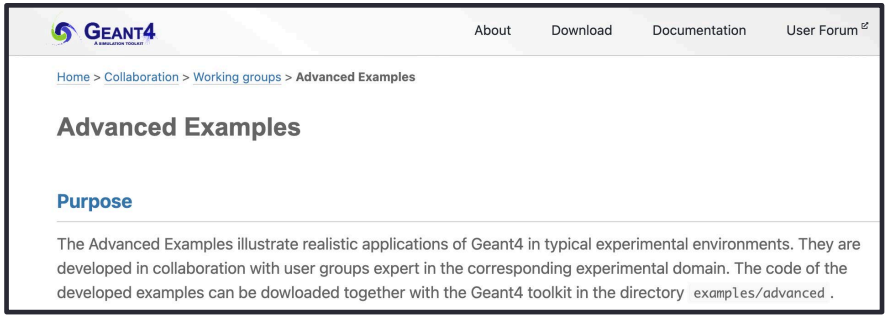
- Definitely a **very successful product**
- Many things changed in >25 years of operation
  - Logo, website, spokesman & coordinators
  - People grew older (and some retired)
- **Participation** by INFN always **significant**
  - Currently, three Steering Board Members

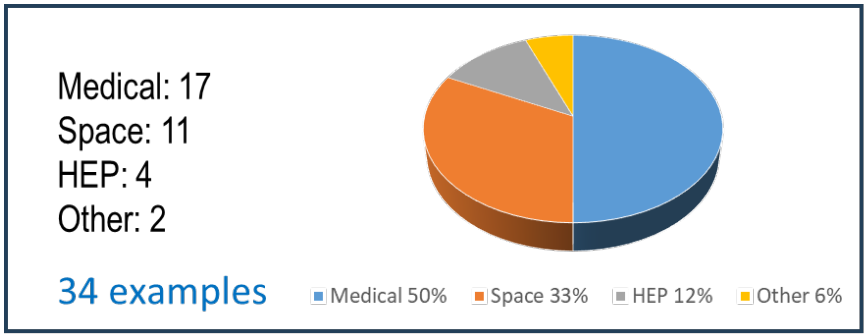
  C. Mancini, F. Romano, A. Sytov

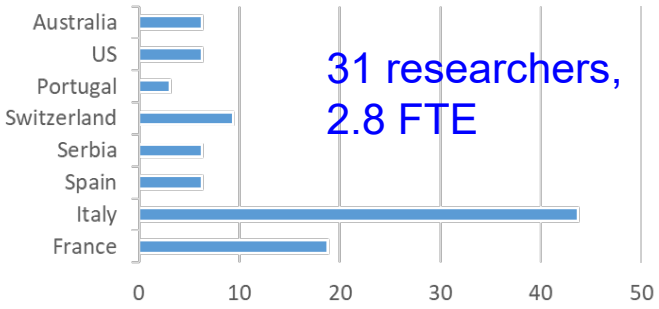


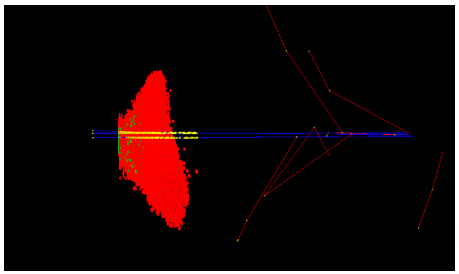
Geant4 advanced examples

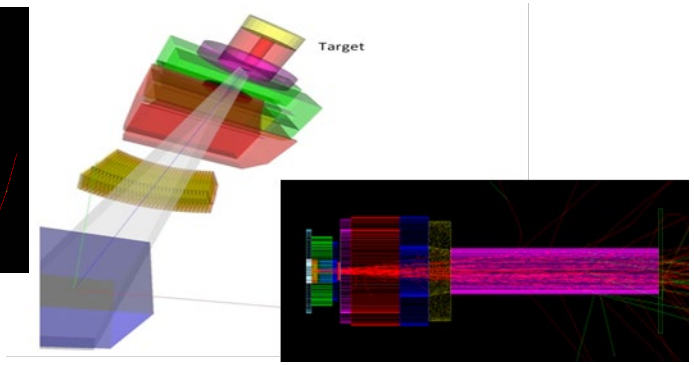
- End-to-end Geant4 **realistic applications** in typical **experimental environments**
  - Strong link with experimental groups → ground for validation!
- Many **different domains** covered (esp. medical & space)
- **Strong involvement** of INFN groups since the beginning









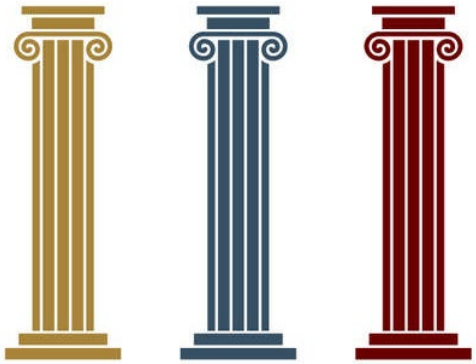


https://geant4.web.cern.ch/collaboration/working_groups/advExamples/

WHAT NOW?

What's still to be done in Geant4?

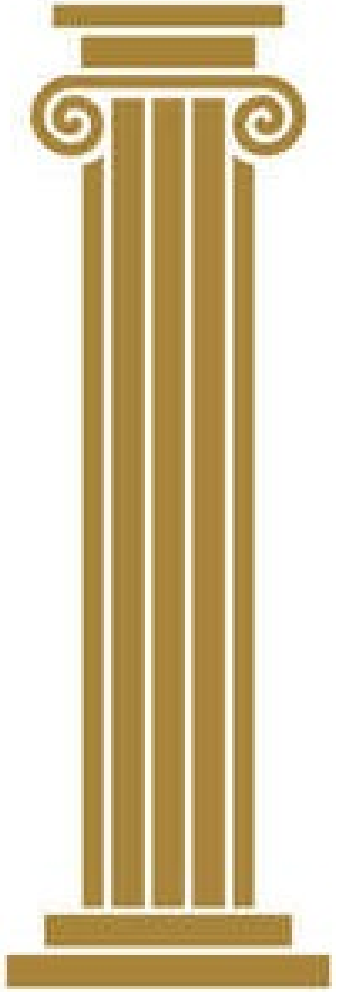
- The *«roaring years»* and the fast developments of the early 2000's are passed
- Now **very stable** and **mature** product
  - Most releases are «minor»: no change in the user interfaces
- **Three key pillars**
  - Development of new physics models
  - Validation
  - Use of novel IT technologies (→ fast development)



- Critical to have an **effective coordination** of the **INFN efforts** within the Geant4 Collaboration
  - Project **Geant4INFN** in CSN5
  - Valorize and maximize the global contribution by INFN
  - Join different communities and provide INFN-wide support

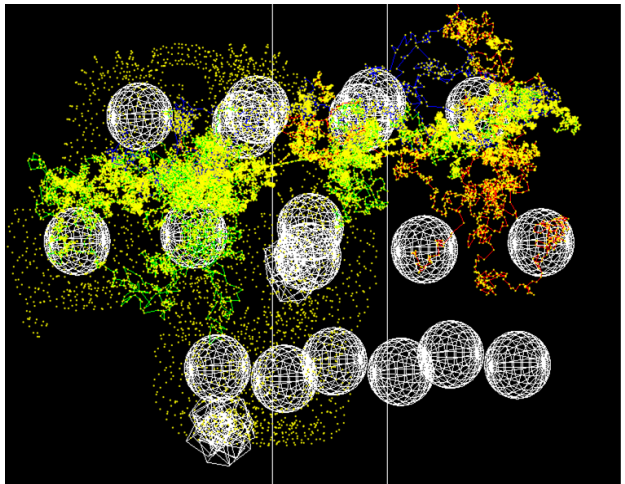
INFN GEANT

NEW MODELS

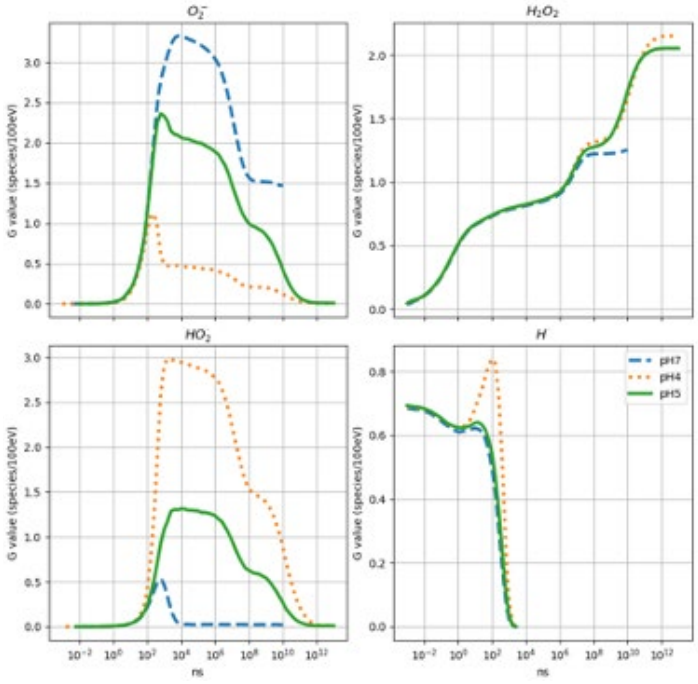


Geant4-DNA

- Simulate interactions at **low-energy** in **biological** materials
  - Follow the physico-chemical and chemical phases
  - Reproduce **quantitatively** cellular damage processes
- **Detailed** simulation (not condensed) → **CPU-intensive**
- In some phases, have to account for secondaries mutual-interaction and chemical equilibrium
- Field of **very active development**
- **Validation** is critical → requires **data**



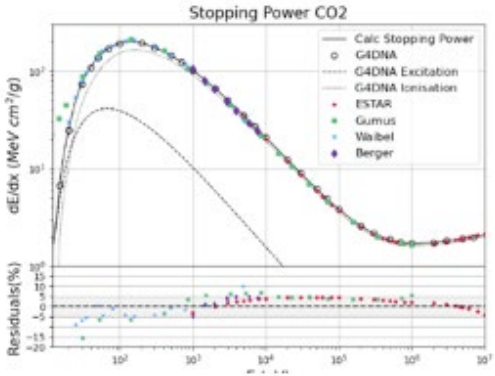
#	Equilibrium	pKa
1	$2H_2O \leftrightarrow OH^- + H_3O^+$	13.999
2	$H_2O_2 + H_2O \leftrightarrow HO_2^- + H_3O^+$	11.65
3	$^{\cdot}OH + H_2O \leftrightarrow O^- + H_3O^+$	11.9
4	$HO_2 + H_2O \leftrightarrow O_2^- + H_3O^+$	4.57
5	$H + H_2O \leftrightarrow e^-_{aq} + H_3O^+$	9.77

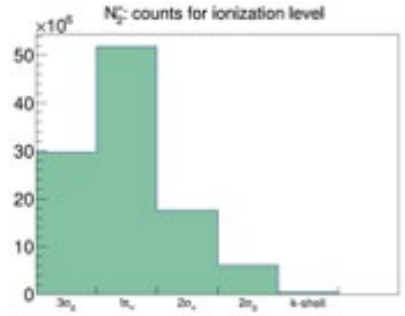


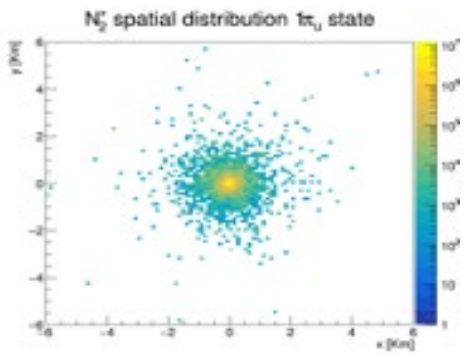
Geant4-DNA extension for atmosphere

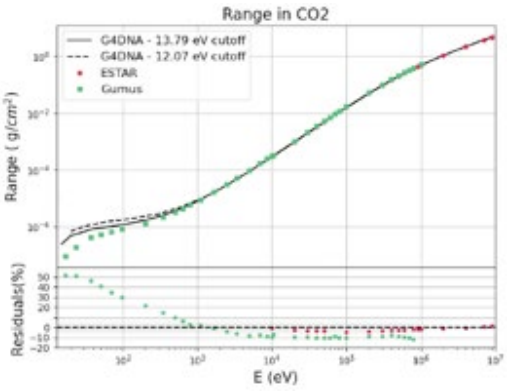
- Important item from **climatology**
  - Cosmic rays are the main source of atmosphere ionisation
  - No MC simulation able to predict ionisation of the medium

- Cross sections for **e- impact** on **N_2, O_2, CO_2** molecules implemented in Geant4-DNA
  - Energy range: 10eV - 10MeV
  - Being extended to positrons
- Three **physics models**:
  - Elastic scattering, Ionization, Excitation
- Check of ranges and stopping powers vs. NIST
- Dissociation process included through the dissociation branching ratios
  - Subsequent **verification** is still needed









Model details: F. Nicolanti, et al, Phys Med. 2023 Sep 11;114:102661.

Model implementations: F. Nicolanti, et al, Accepted by Phys Med. (2024)

Interaction in crystalline materials

- In collaboration with **project Trillion** (Marie Curie Action)

HORIZON 2020

Steering and radiation effects in oriented crystals and their applications implementation into Geant4

- Main goals:
  - Implementation of electromagnetic processes in oriented crystals
  - Specific applications of crystalline effects into Geant4 as extended examples

- **Beam deflection** by a bent crystal
- **Model** and one **example** already released
  - More to come in the next release (3 examples)

A.Sytov et al. J. Korean Phys. Soc. **83** (2023) 132

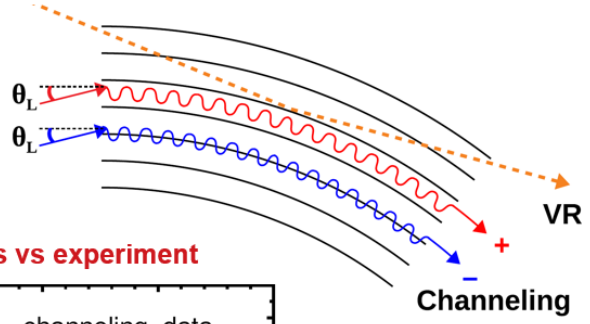
A.Sytov et al. Eur. Phys. J. C **82** (2022) 197

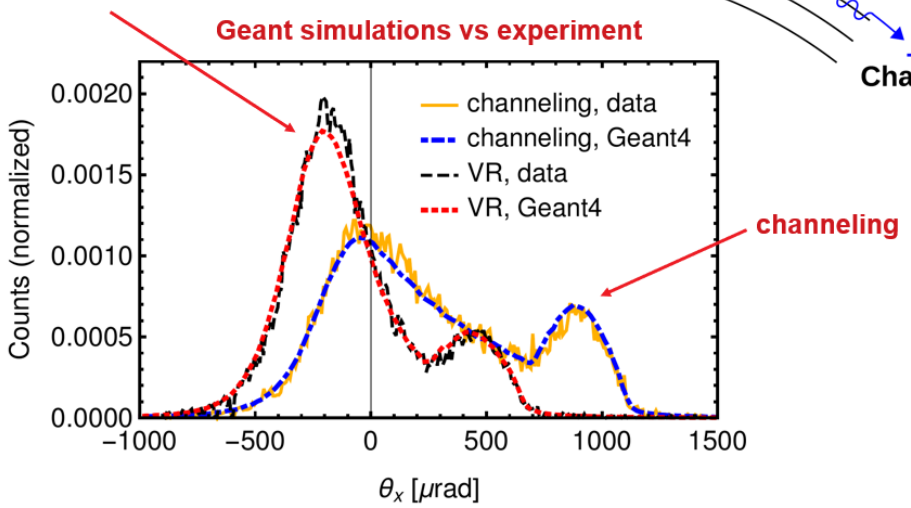
`https://www.fe.infn.it/trillion/`

855 MeV electrons at Mainz Mikrotron

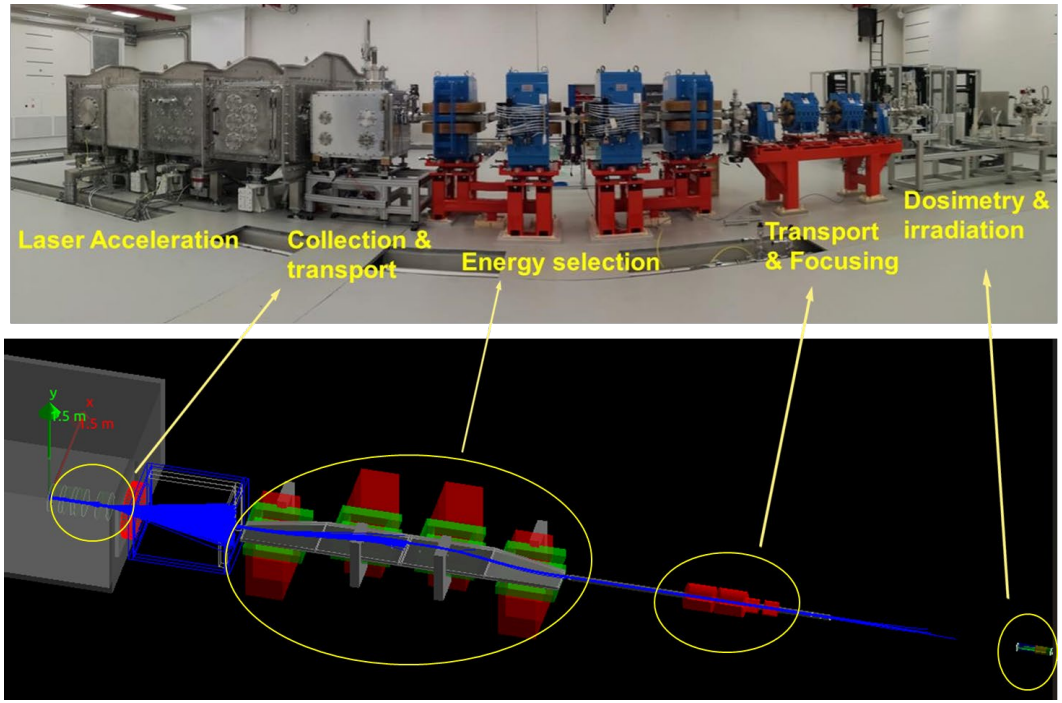
15 μm thick bent crystal

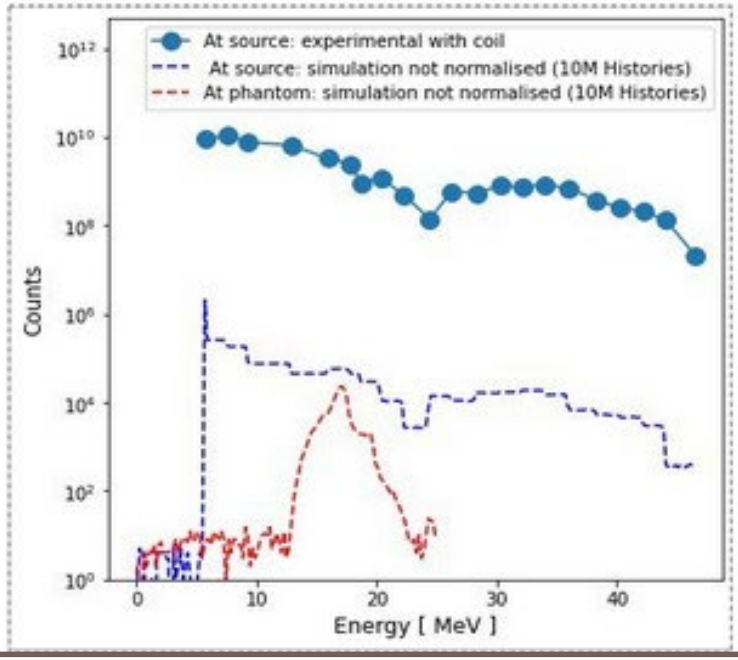
volume reflection (VR)





Laser-driven acceleration





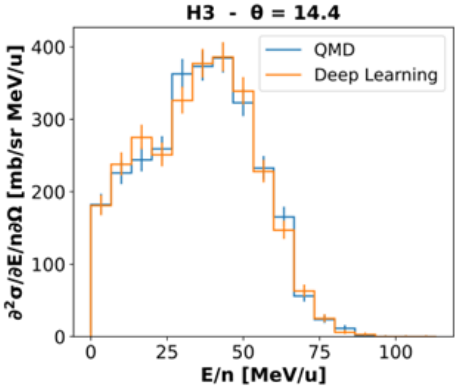
Proton exprimental and simulated spectra generated by the laser interaction on a coil target

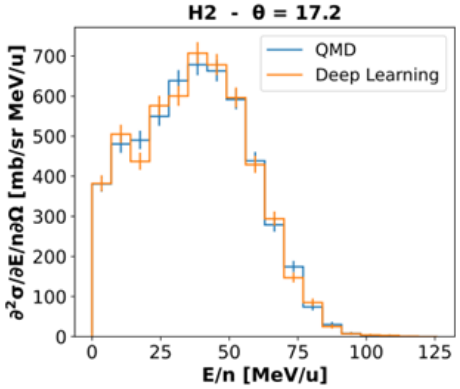
- Goal#1: **reproduce** the outcome from a **laser-driven acceleration beamline**
- Long-term: start to use Geant4 to **simulate laser-plasma interactions**
  - At least in some specific regions of the phase space

Hybrid nuclear interaction models

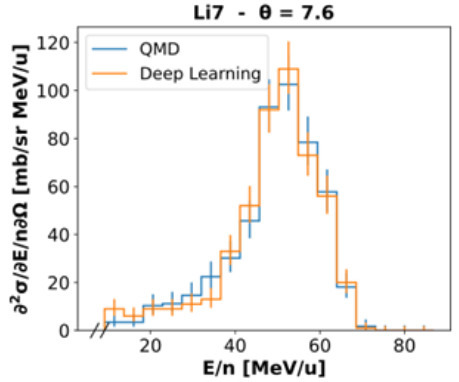
- Accurate models to describe **nucleus-nucleus interactions** at low energy are **very slow**
  - Project GENIALE as «Grant Giovani» fellowship of CSN5
- Exploring the possibility of **accelerating** portion of the model by developing a **physics-informed neural network**

- QMD as a benchmark (possible to apply to LiQMD and BLOB)
- **Emulating** the derivative of the hamiltonian with respect to the generalised coordinates
- **Excellent agreement** with (very slow) MC



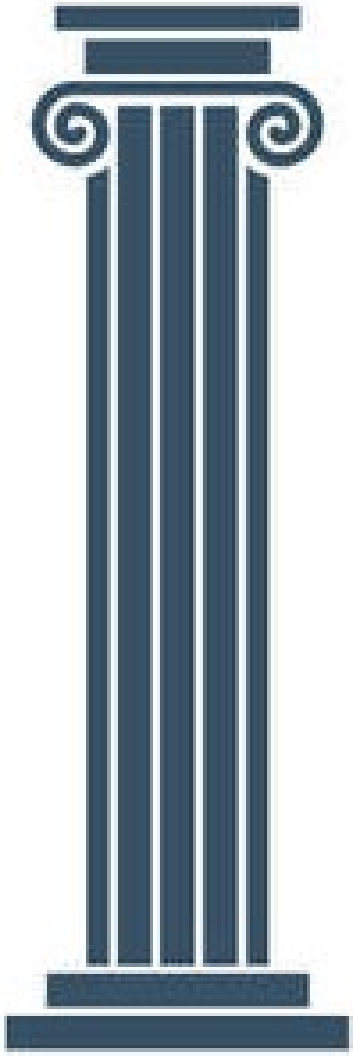


Double differential cross-sections of fragmentation C_{12} on C_{nat} at 62 MeV/u



$$\frac{\partial H}{\partial q, p} \approx \sum A_{ij} + \sum_{\alpha^{(k)}} \left(\sum B_{ij}^{(k)}\right)^{\alpha^{(k)}}$$

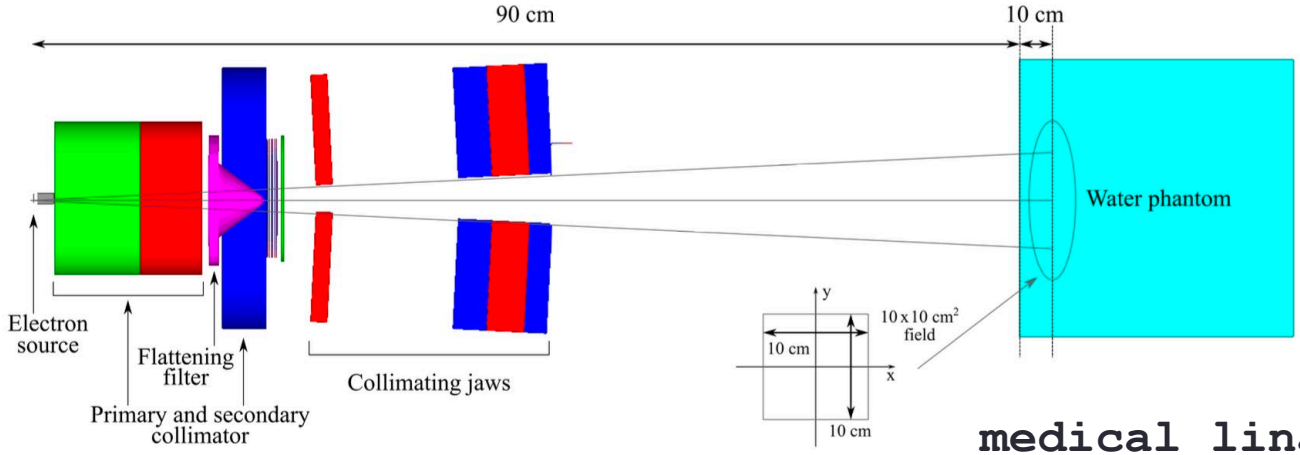
VALIDATION



Medical physics validation (G4Med)

- General project to **benchmark** Geant4 for many **use cases** of **medical interest**
- One paper **published**, one submitted
- Evaluation of the **combination of physics model** of Geant4 which is better suited to reproduce the expeirmental data
  - Different application may require **different physics lists**
- **Several tests/benchmarks** under the **INFN** responsibility
  - E.g. MV X-ray Radiotherapy, validation against EURADOS data

P. Arce et al, Med. Phys. **48** (2021) 19

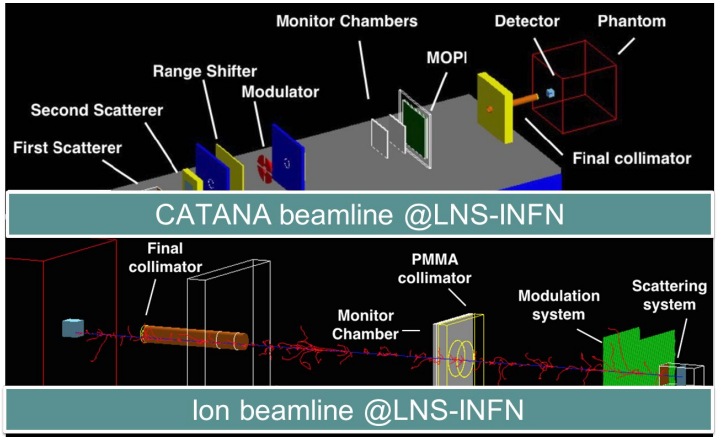


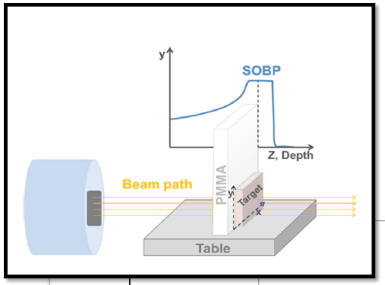
Talk by G. Milluzzo

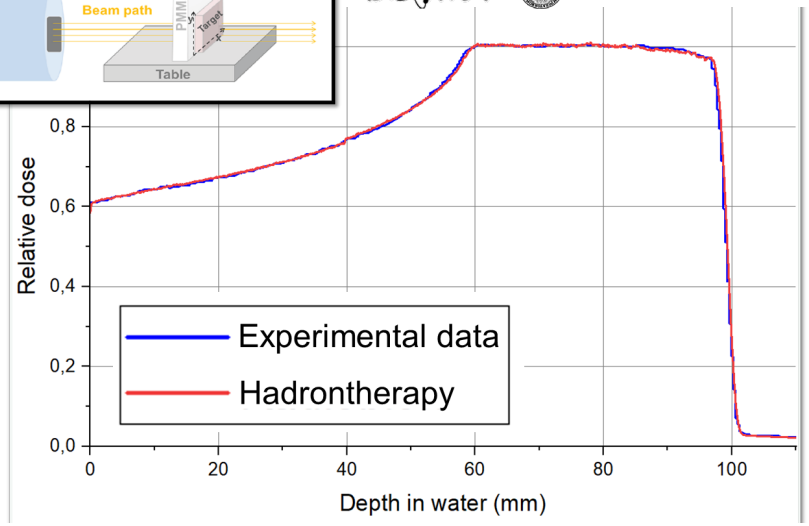
`medical_linac` advanced example

Validation of LET and doses with ion beams

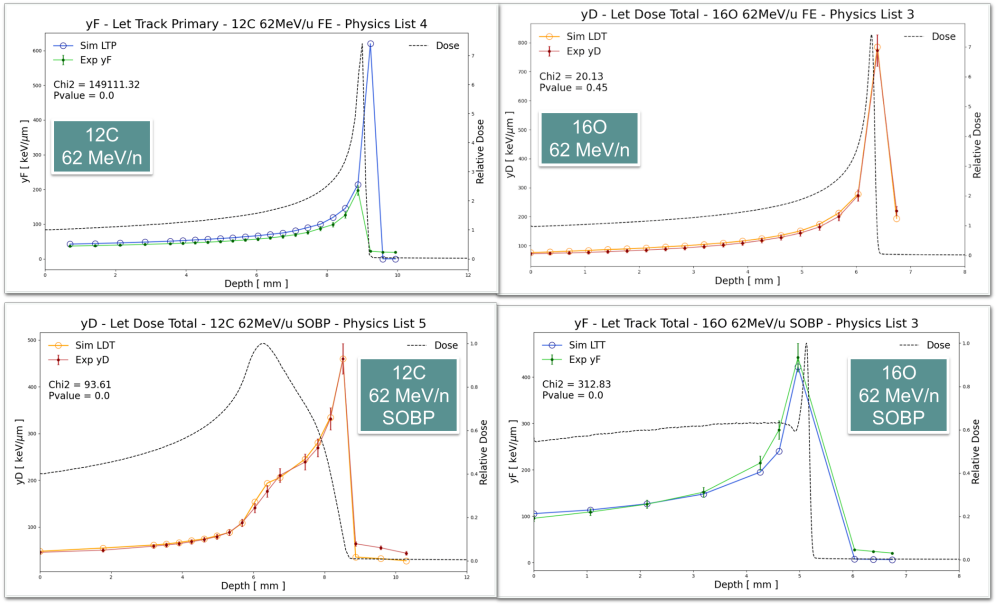
- Advanced example **`hadrontherapy`**
- **Multi-purpose** for several hadrontherapy **beamlines**
- LET and dose space distributions







Five hadronic models: QGSP_BIC; QGSP_BIC_HP; QGSP_BIC_AllHP; GSP_BERT; GSP_BERT_HP



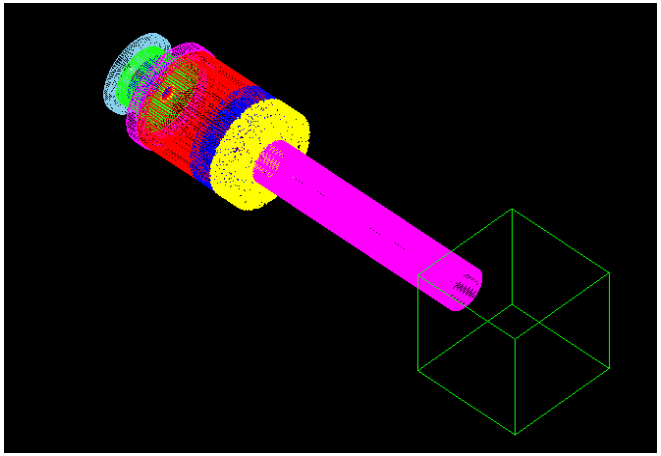
G Petringa *et al* 2020 Phys. Med. Biol. **65** 235043

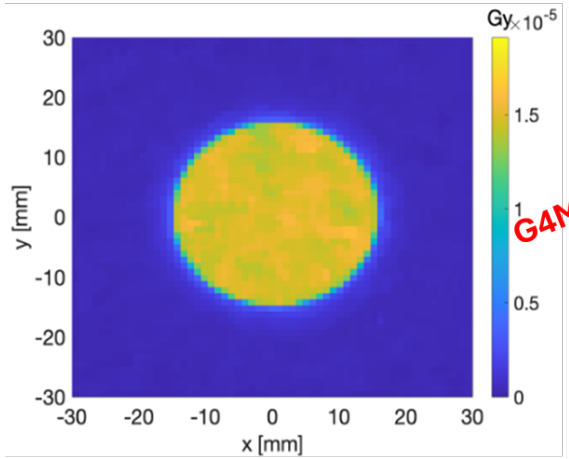
G Petringa *et al* 2021 Appl. Sci. **11** 8822

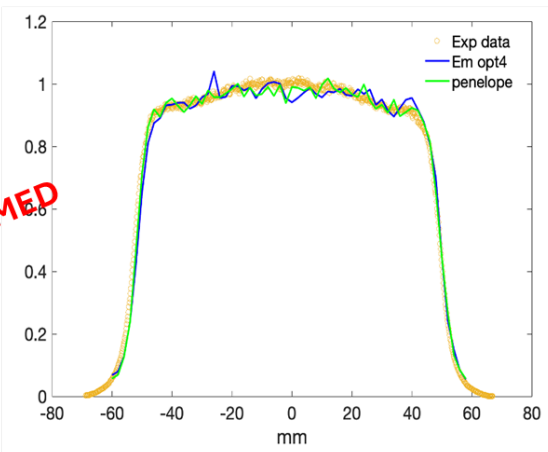
S Fattori *et al* 2022 Phys. Med. Biol **67** 165003

eFLASH therapy

- Dedicated advanced example **`eFLASH_radiotherapy`**
  - Released in Dec 2022
- Simulation of the **ElectronFLASH LINAC** installed at the Centro Pisano for FLASH Radiotherapy
  - Manufacturers' specifications (Sordina Iort Technologies S.p.A)
- Used for **validation** and **benchmarking** within G4Med (dose distributions)







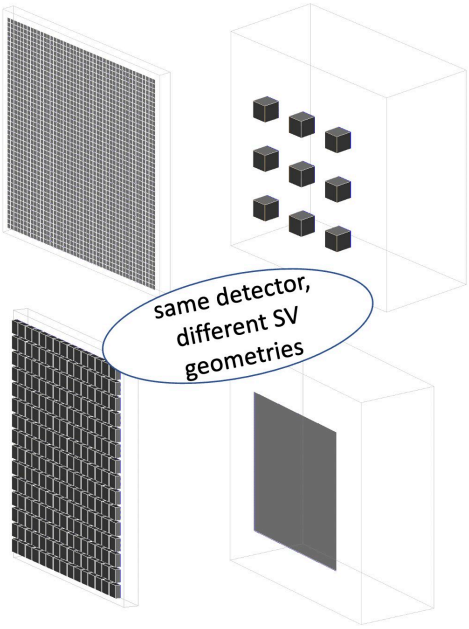
Talk by G. Milluzzo

Microdosimetry

CENTRE FOR MEDICAL RADIATION PHYSICS

INFN CATANIA Istituto Nazionale di Fisica Nucleare Sezione di Catania

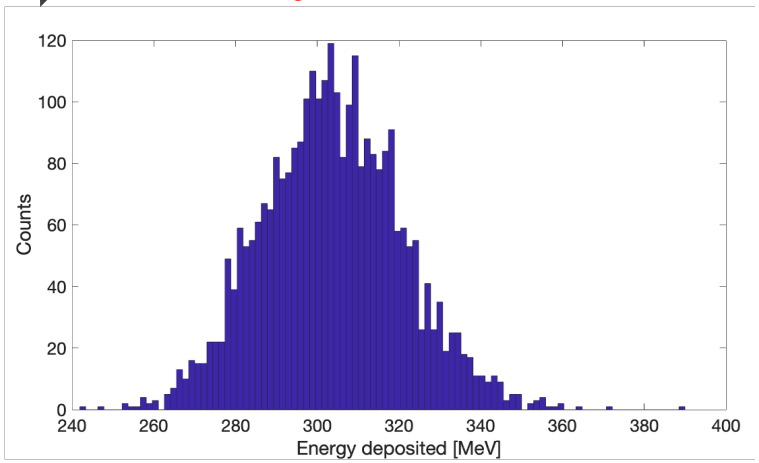
- Recently extended to **clinical** microdosimetric applications (proton and ion therapy)
- **General-purpose** versatile example **`exp_microdosimetry`** for the simulation of several microdosimeters:
  - Silicon, Diamond
  - **TEPC** (*in progress*)
  - **SiC** (*in progress*, see next slide)

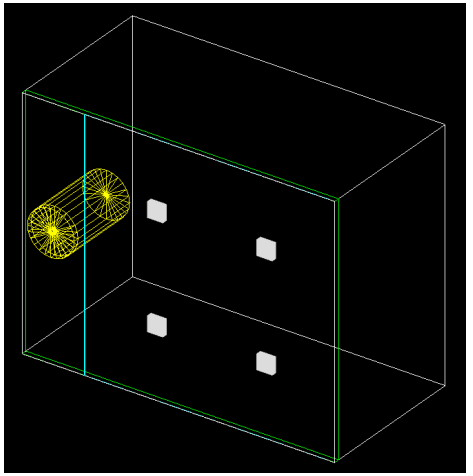


INFN GEANT

- Several **functionalities**
  - Simulation of double-stage geometries for particle identification
- Usable immediately for validation

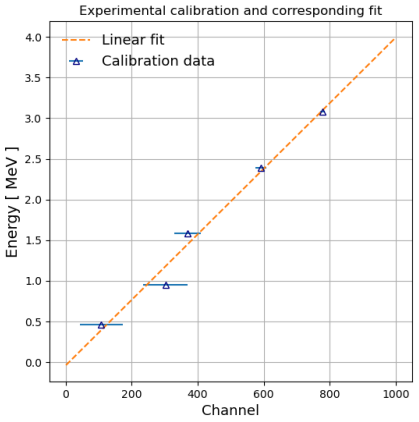
Talk by G. Milluzzo



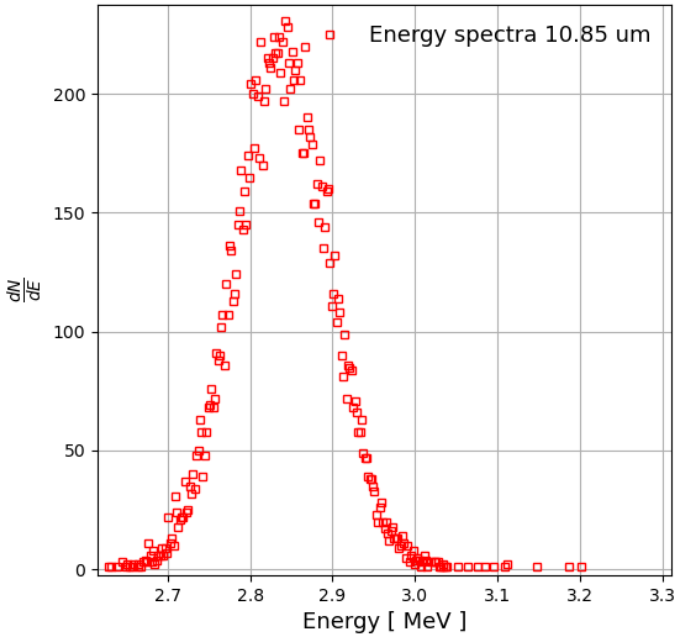


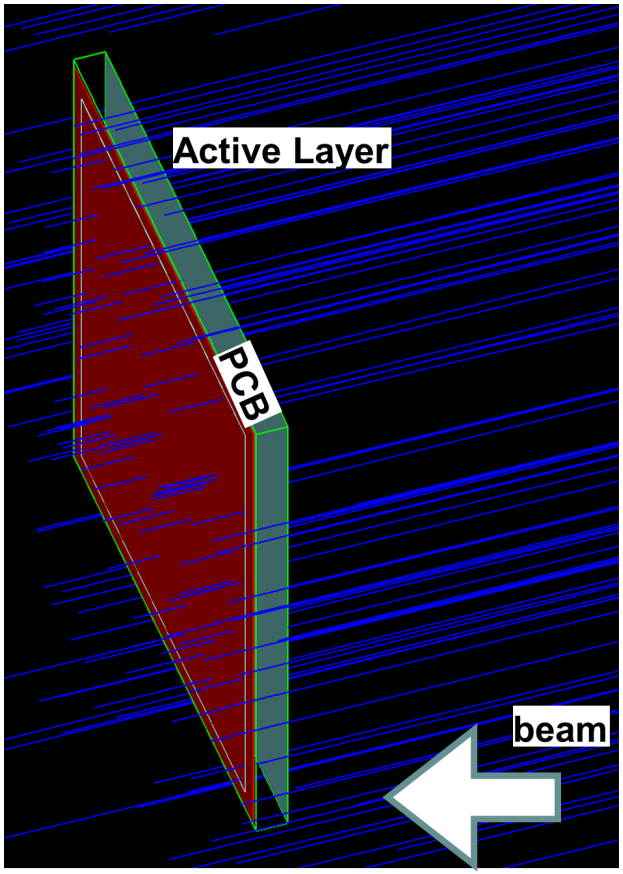
Microdosimetry with SiC detectors

- Dedicated application for a **SiC microdosimeter**
  - Validation of the simulation with dedicated experimental data



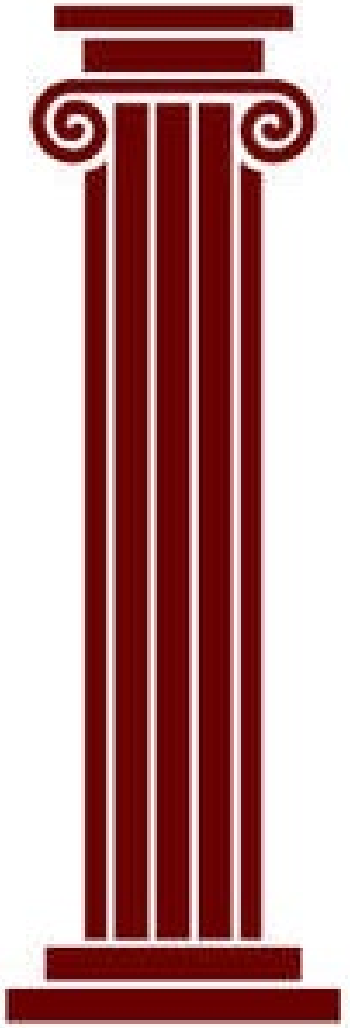
- **Real** detector geometry implemented
  - Passive layers, active layer, electrical contacts...





V Conte *et al* 2020 Phys. Med. Biol. **65** 245018

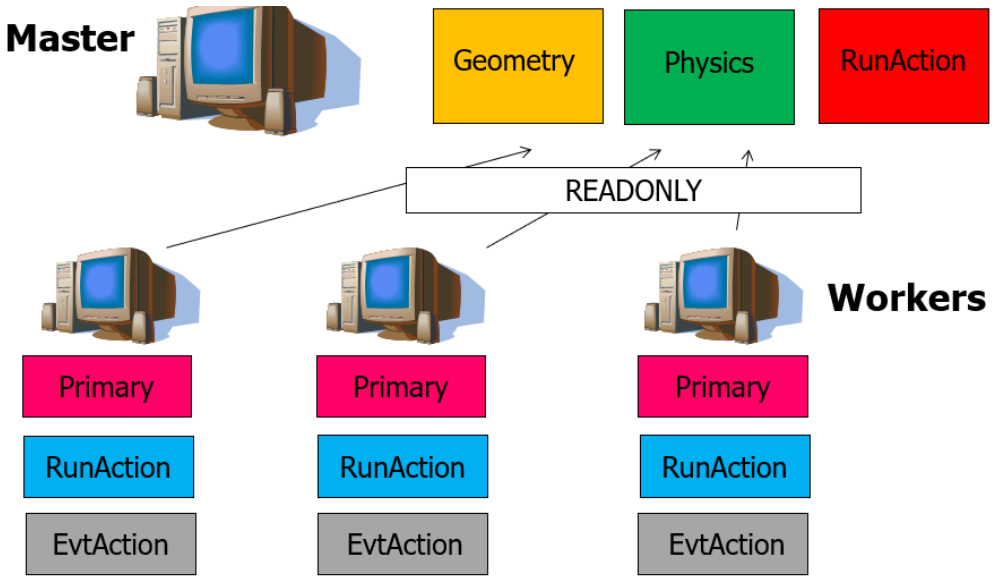
NEW IT TECHNOLOGIES



Catch up with new technologies

- **Rapid evolution** in **IT technologies** (hardware and software)
  - Tools that are «normal» now did not exist in 1998, when the design of Geant4 was worked out and frozen
  - Multi-threading, deep learning, git, cloud, …
- **Geant4** was initially meant to run in «sequential» mode only
  → parallelization (GRID paradigm)

- **Major upgrade** to accommodate for **multi-threading**
  - Available since **Geant4 10.0** (Dec 2013)
  - Share **events** to simulate among different threads
  - **Invasive** changes, painful



Running Geant4 on GPUs

- The particle tracking simulation **not very suitable** for **GPU** implementation (→ parallel tracking)
  - **Very successful** for optical photons (JUNO) and Geant4-DNA (especially for physico-chemical and chemical stages)
- **Several demonstrators** available or **being developed**

J Phys. Conf. Ser. **2438** (2023) 012078

Deferred Optical Photon simulation for the JUNO experiment

Tao Lin (on behalf of the JUNO collaboration)
Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

Med. Phys. **46** (2019) 1483

MPEXS-DNA, a new GPU-based Monte Carlo simulator for track structures and radiation chemistry at subcellular scale

Shogo Okada[a] and Koichi Murakami
KEK, 1-1, Oho, Tsukuba, Ibaraki 305-0801, Japan
Sebastien Incerti
University of Bordeaux CENBG UMR 5797, Gradignan F-33170, France
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(Received 29 July 2018; revised 17 December 2018; accepted for publication 19 December 2018;

- **AdePT** and **Celeritas**:
  - Demonstrators for a full-scale realistic HEP applications (test beams, etc.)
  - EM part ($e^{\pm}$, γ) offloaded to GPU
  - Results compatible with CPU runs
- Geant4 internal «delta» assessment panel in place

J Phys. Conf. Ser. **2438** (2023) 012055

Offloading electromagnetic shower transport to GPUs

G Amadio[1], J Apostolakis[1], P Buncic[1], G Cosmo[1], D Dosaru[2], A Gheata[1], S Hageboeck[1], J Hahnfeld[1], M Hodgkinson[3], B Morgan[4], M Novak[1], A A Petre[5,6], W Pokorski[1], A Ribon[1], G A Stewart[1] and P M Vila[1]
[1] CERN, Geneva (CH)

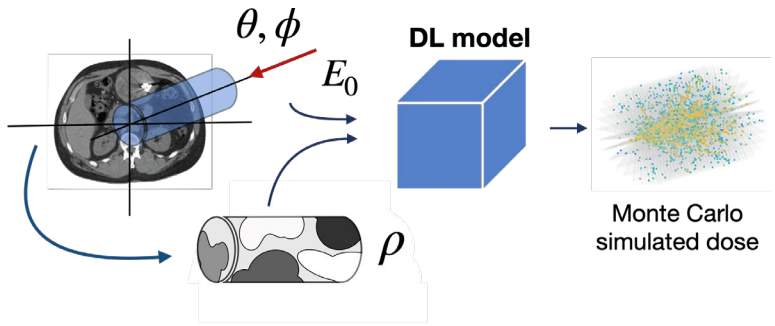
EPJ Web of Conf. **295** (2024) 11005

Celeritas: accelerating Geant4 with GPUs*

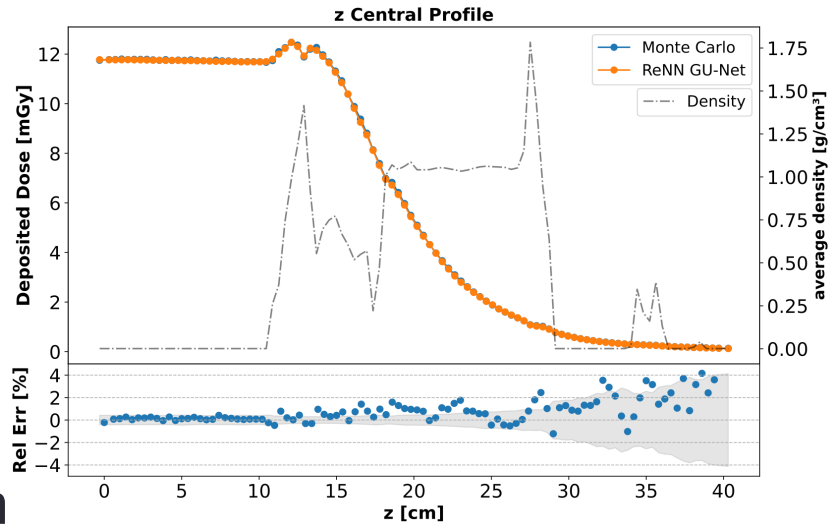
Seth R. Johnson[1,**], *Julien* Esseiva[4], *Elliott* Biondo[1], *Philippe* Canal[2], *Marcel* Demarteau[1], *Thomas* Evans[1], *Soon Yung* Jun[2], *Guilherme* Lima[2], *Amanda* Lund[3], *Paul* Romano[3], and *Stefano* C. Tognini[1]

Machine Learning - Emulation

- **Speed up** CPU-intensive simulations by **emulating** the result of a simulation by a **DL algorithm**
  - Simulation used for training
- Deep Learning Dose Engine



- Developed an algorithm to **emulate dose deposition** as a function of the beam parameters
- **Differentiable** with respect to beam parameters
  - Treatment plan optimization
- Used a Graph Neural Network with a custom pooling technique
- **Cylindrical** geometry around the beam
- **Very good agreement with MC**

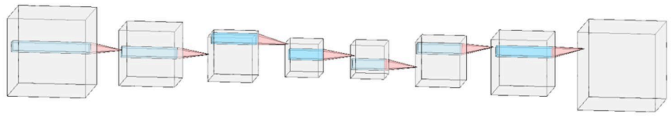


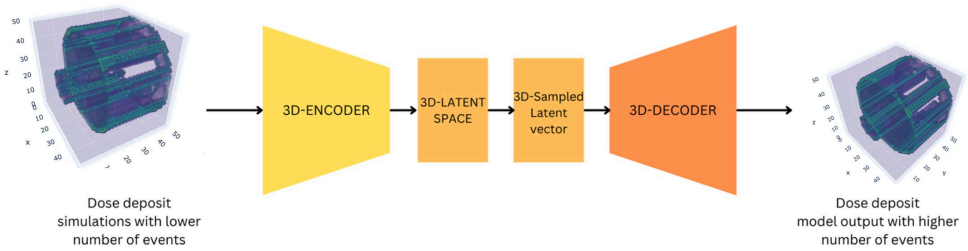
L. Arsini, et al. Algorithms 2023, 16(3)

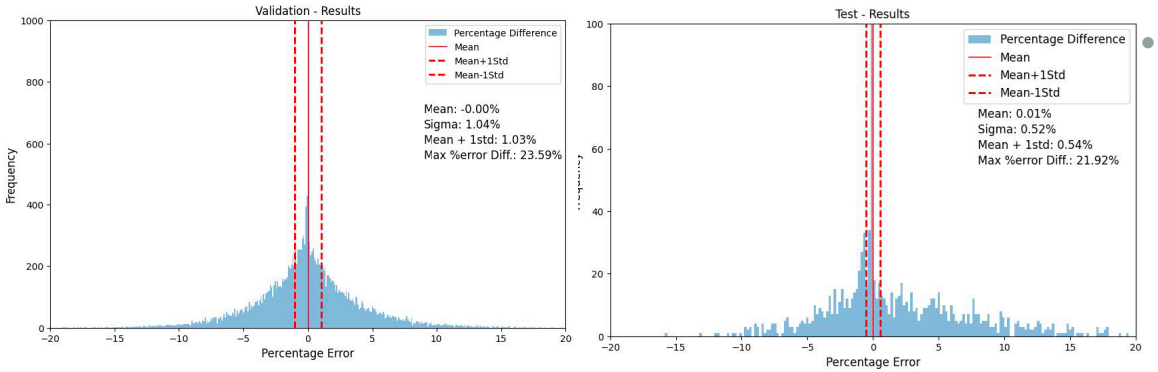
L. Arsini et al. submitted to Frontiers in Physics 2024)

Machine Learning - Super Resolution

- Use ML to **artificially increase** resolution → **MRADSIM**
  - Low-stat sample from MC used for the training





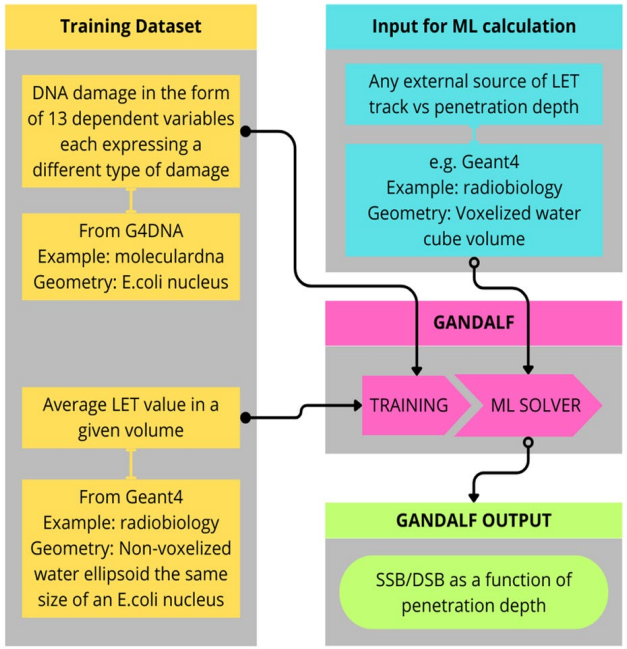


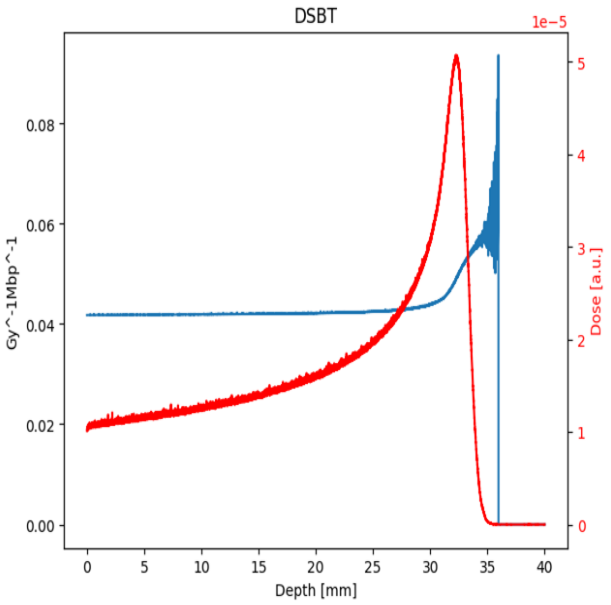
- Created model architecture and tested two different models
  - 3D-VAE
  - Random Forest Regressor
- First tests with limited dataset
- Results are not yet optimized
- **Future** plans:
  - Increase volume and complexity of training dataset
  - Test with different optimizers, loss functions, and other models
  - Increase the number of number of events to predict (up to 10^{12})

Talk by G. Bartolini

Multiscale and machine learning

- Evaluation of the **SSB/DSB damage** by **Geant4-DNA** models very CPU-intensive
- Idea: **bridge the gap**! Train ML to **emulate** this result by using as input the results of a «conventional» (and much faster) Geant4 simulation (dose, LET, RBE, …)
  - Extended example **`radiobiology`** very suitable
- **GANDALF**: **G**enerative **AN**satz for **D**NA damage ev**AL**uation and **F**orecast
  - Neural Network regression system trained with a mixed dataset from Geant4 and Geant4-DNA



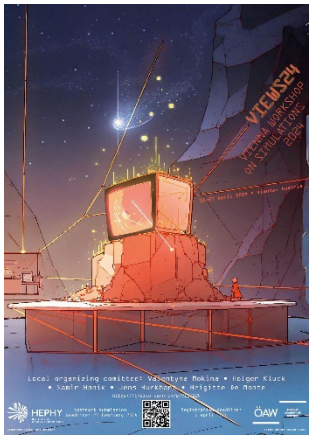


Containers and Cloud

- Pack a fully working **Geant4 installation** in a **container**
  - Deployment everywhere, as a **docker image**
- Use **Apptainer** (formerly Singularity)
  - Compatible with Docker images
  - Largely available on scientific computing clusters
- With a few commands it's possible to **run a Geant4 application** regardless of the environment (even without installing Geant4)
  - The container is built via GitHub CI and hosted on GitHub itself
- **Multiple use-cases**:
  - Validation jobs (e.g. split in many locations) → G4val, G4med
  - Training (e.g. Geant4 courses)
  - Cross-platform portability

Training

- Intense activity within **INFN** for **dissemination and training** on Geant4
  - Recently extended to Geant4-DNA (dedicated path)
  - Coordinated by Geant4INFN
- Targeting **scientific users** (PhD, postDocs, …) in all fields of interest of **INFN**, but participants also from **companies**
- **Four** courses in 2024
  - XI International Geant4 School (January, Pavia)
    - w/ Geant4-DNA
  - VIEWS Workshop (April, Vienna)
  - Alghero Seminar (June, Alghero)
  - XII International Geant4 School (November, Bucarest)
    - w/ Geant4-DNA



XI International Geant4 School

14–19 Jan 2024
University of Pavia, Physics Department
Europe/Rome timezone

The XII Geant4 International School

25–29 nov 2024
Extreme Light Infrastructure - Nuclear Physics (ELI-NP)
Europe/Bucharest fuso orario

A quick summary

- Geant4 is a **mature software**, widely used in a variety of physics domain of interest for INFN
- **INFN strongly involved** in the development since the beginning
  - Interesting for applied physics and for technological transfer
- Despite the maturity, **quite a lot of activity**
  - Development of physics models in innovative domains and directions
    - Geant4-DNA, crystals, laser, N-N
  - Validation and QA/QC, especially in medical physics
    - Strong synergy with experimentalists
  - Efficient use of opportunities by novel IT technologies
- **Geant4INFN** project in CSN5 acting as the **collector** of the **Geant4 activities** within INFN
  - Optimize the global contribution to Geant4 by INFN
  - Offer support (+ training) to the INFN community