Codici Monte Carlo in Fisica Medica

Esempio dettagliato: FLUKA e le sue applicazioni in radioterapia e adroterapia

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Analog versus condensed history MC

Condensed history MC simulation

- Many "small-effect" (*"soft"*) interactions can be grouped into few condensed history "steps"
- Sample of the cumulative effect from proper distributions of grouped single interactions (multiple scattering, stopping power,…)
- *"Hard"* collisions (e.g., δ-ray production) can be explicitly simulated in an analog matter

Example of e^- track

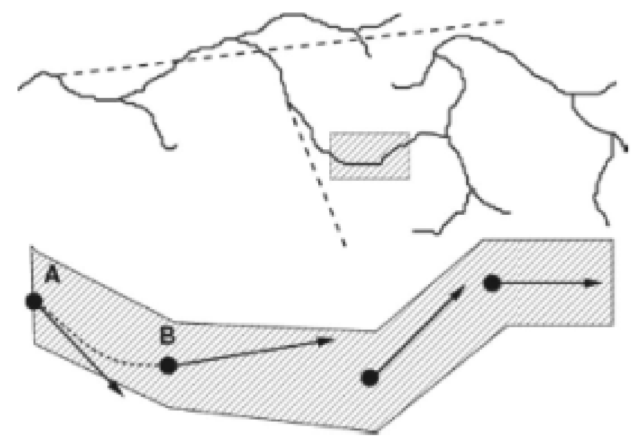


FIG. 1. Illustration of a class II condensed history scheme for electron transport. The upper portion shows a complete electron track including secondary electrons and photons (shown with dashed lines and not including their interactions) with energies above the hard collision thresholds. The lower portion is a magnified view of the shaded box.

I Chetty et al, Report of the AAPM Task Group 105, Med Phys 34, 2007

Approach followed in all general purpose MC codes

General Purpose Codes (condensed history) applied to Medical Physics

PENELOPE (electrons/positrons/photons)

FLUKA

MCNP (mostly for neutrons
→ Boron Neutron Capture Therapy)

GEANT4
- GATE
- TOPAS
- GAMOS
- ....

MC Codes (condensed history) dedicated to specific medical applications (Hadrontehrapy)

PHITS

SHIELD-HIT

Penelope

Penetration and ENErgy LOss of Positrons and Electrons

50 eV – 1 GeV

Used for: Dose Calculation, X-Ray tube modelling, Beam Modelling

Notice: cross sections provides for energies underneath 1 keV are subject to large uncertainties which is also true for other codes that claim to simulate transportation down to such low energies

Addiotional tool **PENGEOM**: flexible geometry tool, which allows for automatic particle tracking in complex geometries.

The OECD/NEA Data Bank distributes the PENELOPE software.

NEA (2019), ***PENELOPE 2018: A code system for Monte Carlo simulation of electron and photon transport***, *Workshop Proceedings, Barcelona, Spain, 28 January – 1 February 2019*, OECD Publishing, Paris, https://doi.org/10.1787/32da5043-en.

MCNP

Monte Carlo N-Particle

1 keV – thousands of TeV
34 similar kinds of particles and about 2000 ions.
Used for dose Calculation, Shielding, Beam Modelling, particle tracking - transport through matter, BNCTetc

Developed at Los Alamos National Laboratories, is one of the most important general purpose three-dimensional MC codes. It is well known in nuclear physics and used for studies including criticality, shielding, and detector response, but also dosimetry and many other applications, including medical ones.
Pointwise cross-section data typically are used, although group-wise data also are available. For neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B-VI) are accounted for. Thermal neutrons are described by both the free gas and S(alpha,beta) models. Rich collection of variance reduction techniques; a flexible tally (=scoring) structure and an extensive collection of cross-section data.

T. Goorley et al. Initial MCNP6 release overview MCNP6 version 0.1. Nucl Technol. (2012). 180:298–315.

https://mcnpx.lanl.gov/

GEANT4

50 eV – thousands of TeV

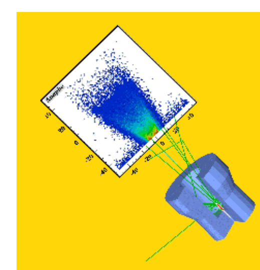
Mainly used for development of Software packages, core toolkit.

GEANT (GEometry ANd Tracking) software toolkit that encapsulates modern design and state of art developing techniques using Monte Carlo modelling methods to explain the movement of elementary particles through matter.

The base of Geant4 is a plenty set of physics models to take care of particle-matter encounters covering a large area of energy range. In few words we can say that the software toolkit encapsulates information and modelling methods used from many sources around the world.

Notice: Penelope is imported in **GEANT4** a e.m. physics package

P. Arce, et al., ***Report on G4-Med, a Geant4 benchmarking system for medical physics applications developed by the Geant4 Medical Simulation Benchmarking Group****, Medical Physics, 48, n. 1 (2021) 19-56*
https://doi.org/10.1002/mp.14226



https://geant4.web.cern.ch/

GATE

Geant4 Application for Emission Tomography)

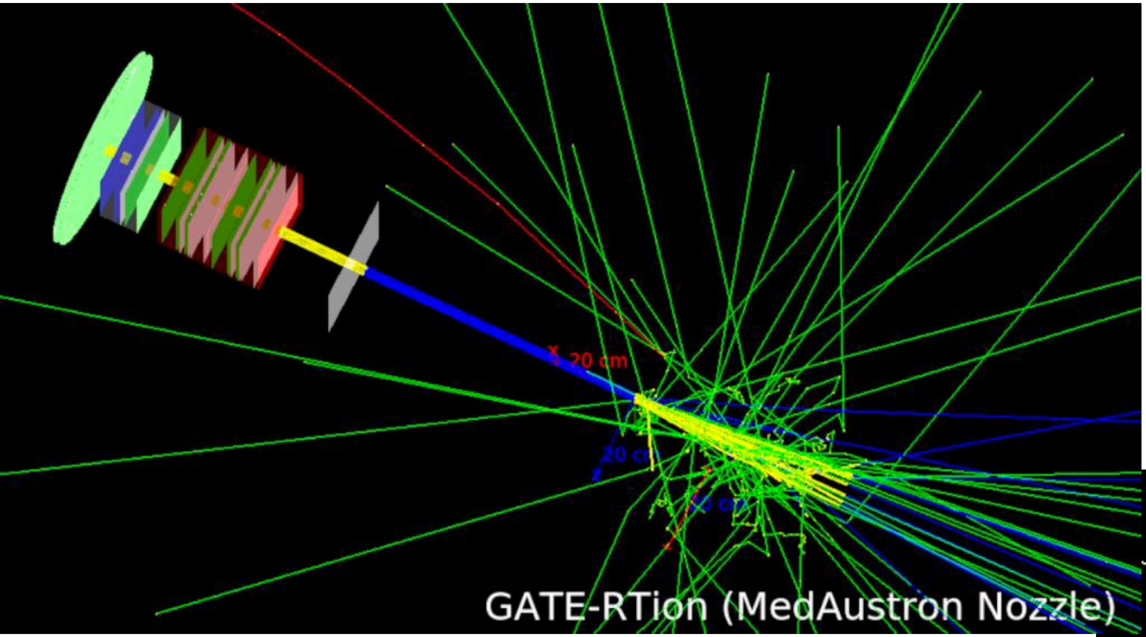
50 eV – thousands of TeV
Hadrons, electrons, photons, positrons, can implement geant4 particles
Used for PET, SPECT, CT, Radiotherapy, Dosimetry, Proton Therapy, Thermal Therapy, etc

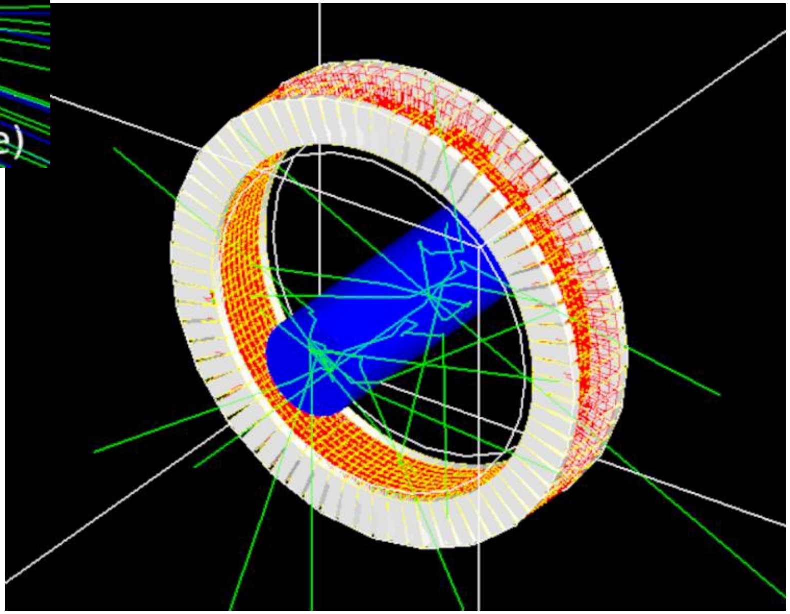
GATE is a software package that combines photographs, radiotherapy, and dosimetry in one environment. It was created to conduct experiments with PET and SPECT.
Since 6.0 version, new software has been introduced devoted to radiation therapy simulations, including linear accelerator simulations .
GATE utilizes the GEANT4 toolkit classes to provide a scalable, flexible scripts for computational experimentation in nuclear medicine. In particular the software allows the modelling phenomena of electronics and mechanical parts of the detector.

D. Sarrut, et al., "A review of the use and potential of the GATE Monte Carlo simulation code for radiation therapy and dosimetry applications" Medical Physics, 41 (2014) https://aapm.onlinelibrary.wiley.com/doi/full/10.1118/1.4871617

http://www.opengatecollaboration.org/

GATE
Geant4 Application for Emission Tomography





GAMOS

Geant4-based Architecture for Medicine-Oriented Simulations

Hadrons, electrons, photons, positrons, can implement geant4 particles
50 eV – thousands of TeV
Used for PET, SPECT, Compton Camera, Shielding, Radiotherapy, etc.

GAMOS is a MC emulation platform built on the Geant4 toolkit, with the exception that it is more user-friendly and more scalable than GEANT4.
It allows inexperienced people make experimentations and build their project without bothering to write in C++. It requires just a basic understanding of **Geant4.**
The scripting language of **GAMOS** makes it simple to implement the most basic specifications capable of reproducing Medical Physics experimentation.
The plugin technology, together with a modular architecture, extensive documentation, and a series of examples and tutorials, helps users to fully leverage **GEANT4**'s functionality by writing new user code or reusing existing **GEANT4** code and combining it seamlessly with existing **GAMOS** modules.

http://fismed.ciemat.es/GAMOS/gamos_publications.php

TOPAS

TOol for PArticle Simulations

Hadrons, electrons, photons, positrons, can implement geant4 particles

50 eV – thousands of TeV

Used for Linacs, Proton therapy, Dose calculations, Radiotherapy

TOPAS bundles and expands the Geant4 libraries to take advantage of a more sophisticated Monte Carlo simulation which includes most types of radiotherapy available systems so that medical physicists can find it more easily to use.

TOPAS can emulate effectively photon and particle therapy systems, build a human geometry from CT DICOM pictures, score doses, calculate fluence, and other parameters

Though proton therapy was the most common early use of **TOPAS**, it is now accessible for usage in all radiation treatment domains, as well as some medical imaging applications. **TOPAS** is currently being expanded to include radiation biology (see later) and scientific education.

http://www.topasmc.org/

SHIELD-HIT

SHIELD-HIT12A is a Monte Carlo particle transport program which is modified for proton and heavy ion particle therapy reserach. It was forked from SHIELD-HIT in 2008 with the aim to modernize and implement new features, increasing the applicability for medical physics.

N Bassler et al 2014 J. Phys.: Conf. Ser. 489 012004

DC Hansen, A Lühr, R Herrmann, N Sobolevsky, N Bassler; Recent improvements in the SHIELD-HIT code; International Journal of Radiation Biology, January 2012, Vol. 88, No. 1-2 , Pages 195-199;

David C Hansen, Armin Lühr, Nikolai Sobolevsky and Niels Bassler; Optimizing SHIELD-HIT for carbon ion treatment; Physics in Medicine and Biology, 2012, Vol. 57, No. 8, Pages 2393

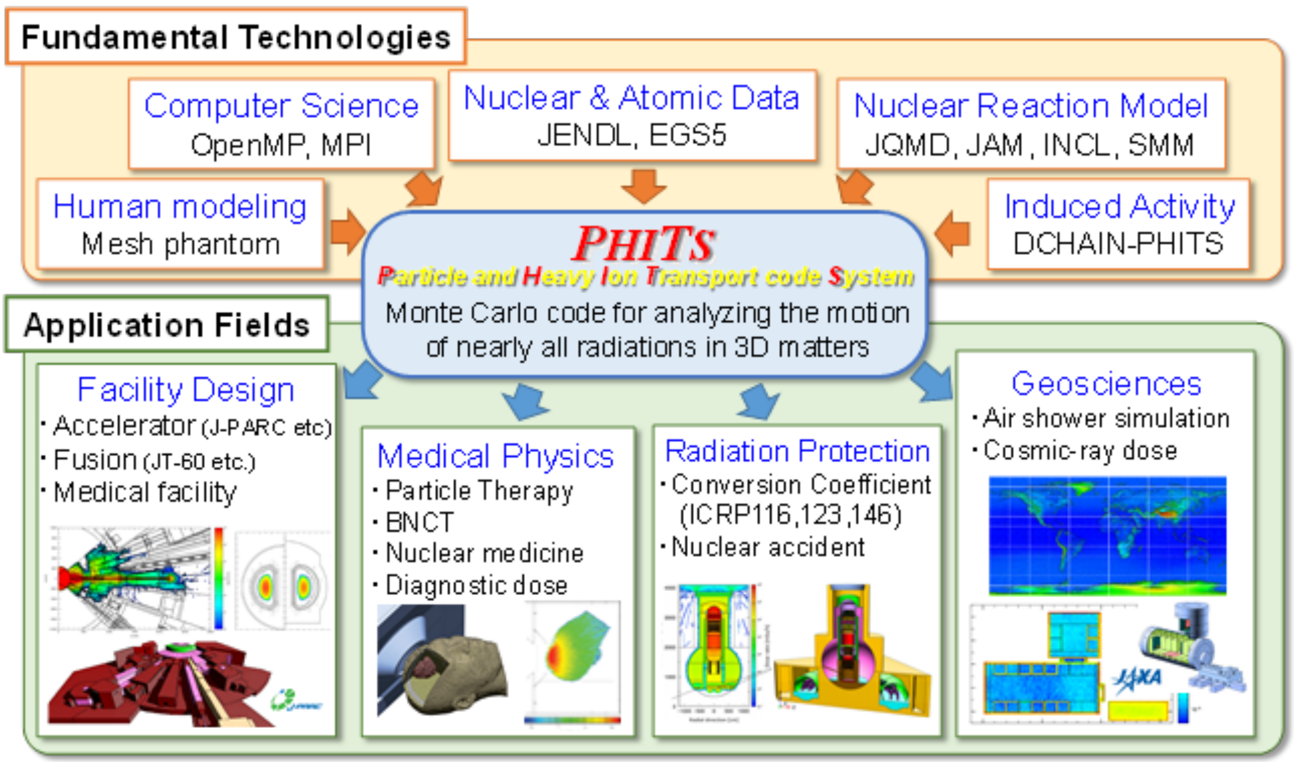
https://shieldhit.org/

PHITS

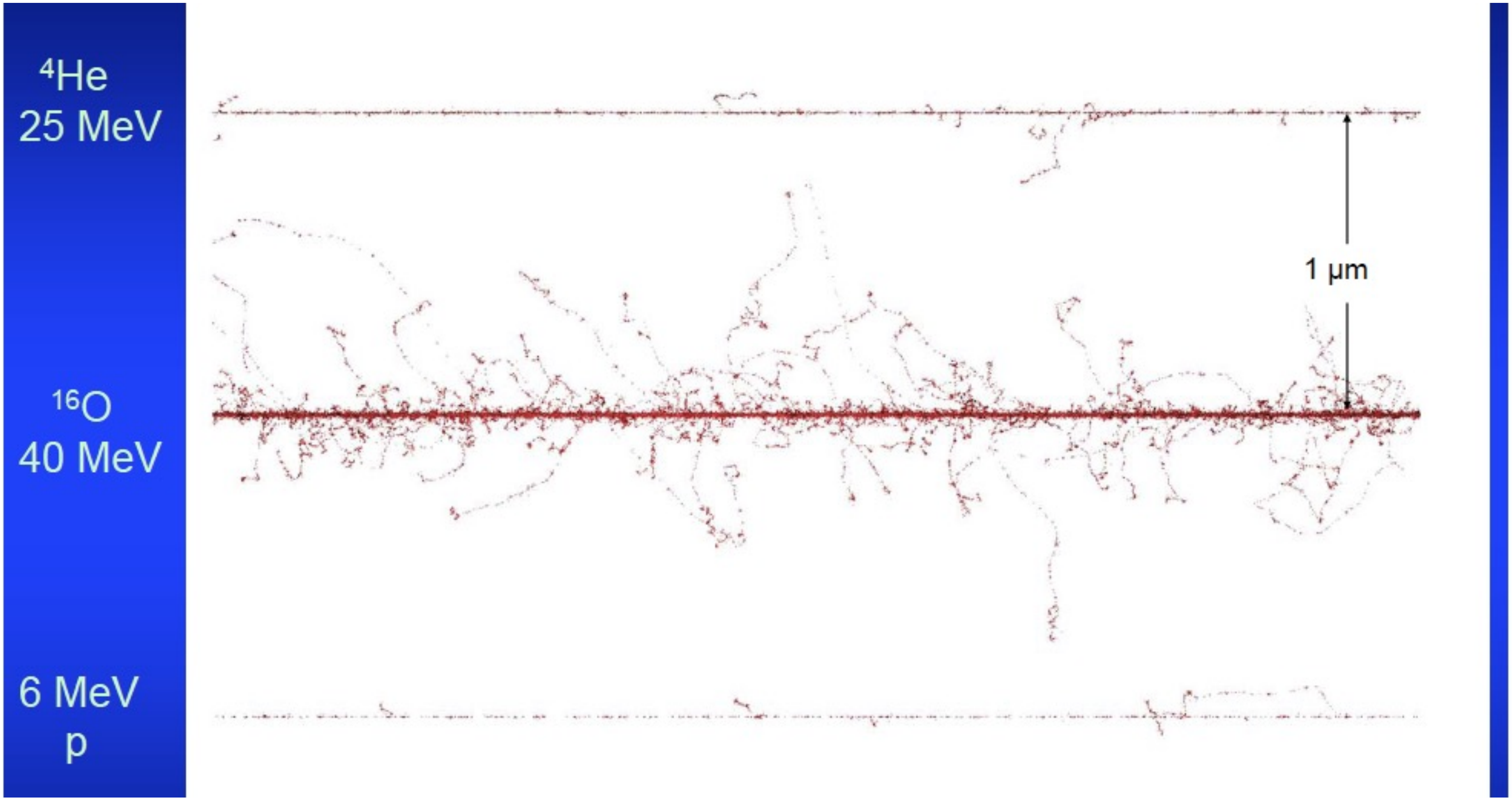
Particle and Heavy Ion Transport code System

https://phits.jaea.go.jp/

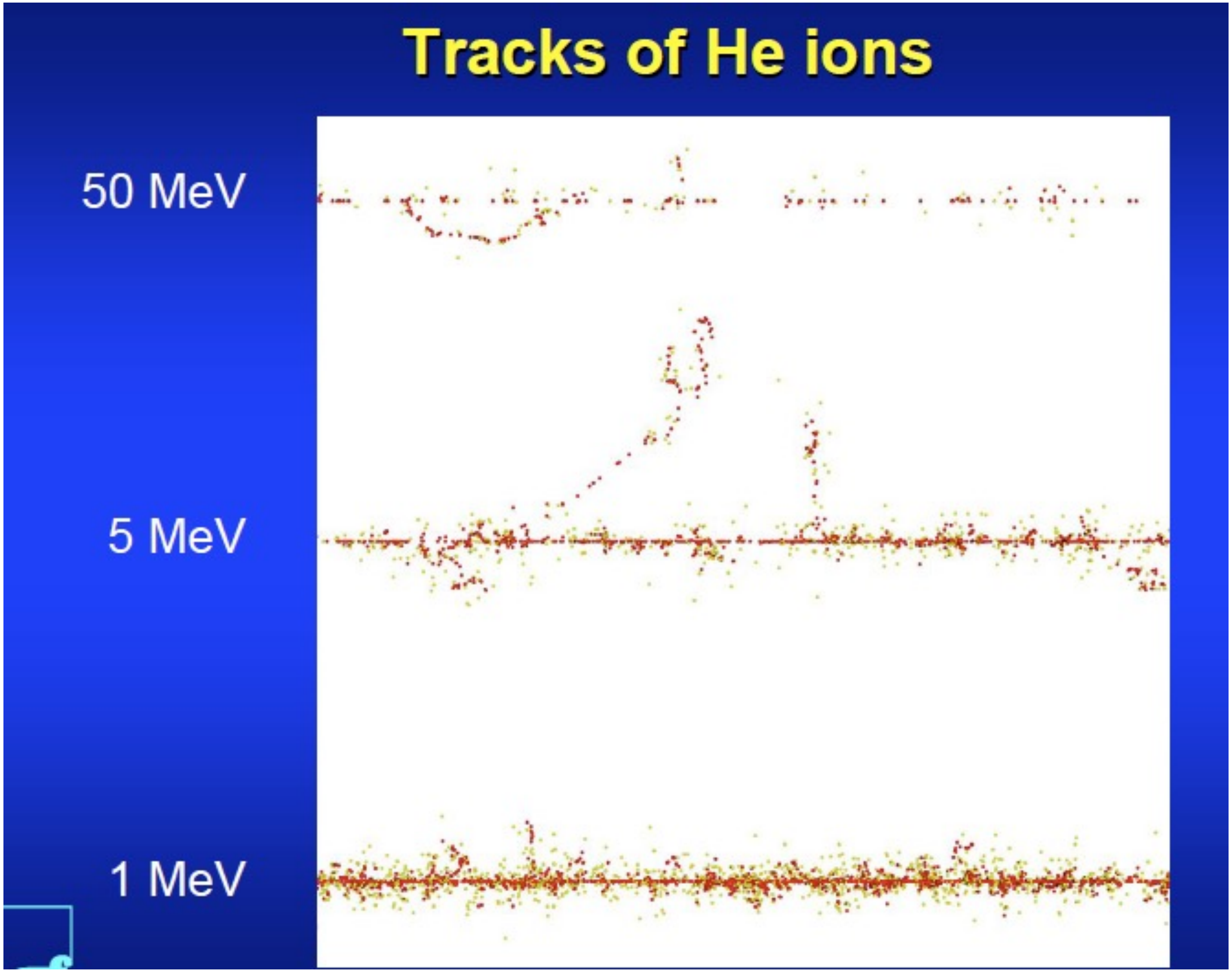
PHITS (Particle and Heavy Ion Transport code System) is a general purpose Monte Carlo particle transport simulation code developed under collaboration between JAEA, RIST, KEK and several other institutes. It can deal with the transport of all particles over wide energy ranges, using several nuclear reaction models and nuclear data libraries.



Track Structure MC - 1



Track Structure MC - 2



Track Structure codes - 3

Track structure codes are in general able to perform calculations on microscopic (nanometric) volume scales in liquid water, making their application in simulations of actual clinical cases highly unpractical from the point of view of computing power.

However, they remain fundamental, together with mathematical models of the cell structure, for the investigation of all basic mechanisms related to biological effects of radiation.

PARTRAC: performs calculations on microscopic scales in liquid water
*M. Dingfelder et al.. **Electron inelastic-scattering cross sections in liquid water.** Radiat Phys Chem. (1998). 53, 1–18.*

TRAX: can deal with different materials.
Wälzlein C, Krämer M, Scifoni E, Durante M. Advancing the modeling in particle therapy: from track structure to treatment planning. Appl Radiat Isot. (2014). 83:171–6.

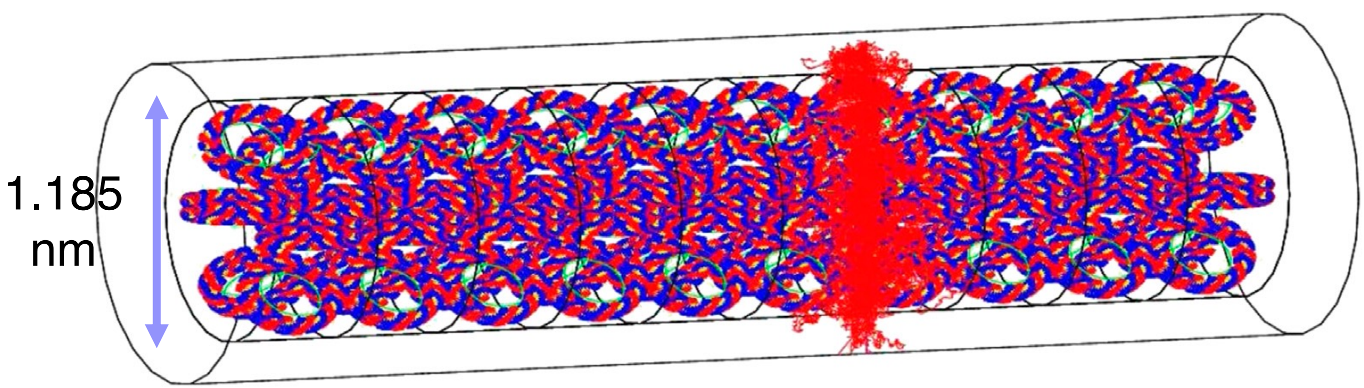
Results obtainable by these codes can in principle be coupled with the radiation field simulation achievable with general purpose MC codes.

Track Structure codes -3

GEANT4-DNA: It was started in the context of the studies for radiation protection in space missions. The code currently includes the interactions of light particles (electrons) and ions including hydrogen and helium isotopes down to the eV scale in liquid water.

http://geant4-dna.org/

It allows to implement the geometry of biological targets at submicrometric scales. Tt can use either a voxelized or an atomistic approach. The latter allows to model targets at nanometric scales, such as the DNA molecule, using the combination of standard mathematical volumes.



Visualization of a whole chromatin fiber irradiated by a single 500 keV He+ particle,

*S. Incerti et al., **The GEANT4-DNA project**. Int J Model Simul Sci Comput. (2010). 1. 157–78.*

A chemistry model can be coupled to simulate indirect radiation effects

Track Structure codes - 4

TOPAS has an extension was developed called **TOPAS-nBio**, which is aimed at the modeling of detailed biological effects at the nanometer scale, facilitating and extending the use of **GEANT4-DNA** models for subcellular geometries, physics, and chemistry processes.

J. Schuemann et al., TOPAS-nBio: an extension to the TOPAS simulation toolkit for cellular and subcellular radiobiology. Radiat Res. (2019). 191, 25–38.

https://gray.mgh.harvard.edu/research/software/258-topas-nbio

Un esempio di Codice Monte Carlo e di sua applicazione in Fisica Medica:

FLUKA e le sue applicazioni in radioterapia e adroterapia

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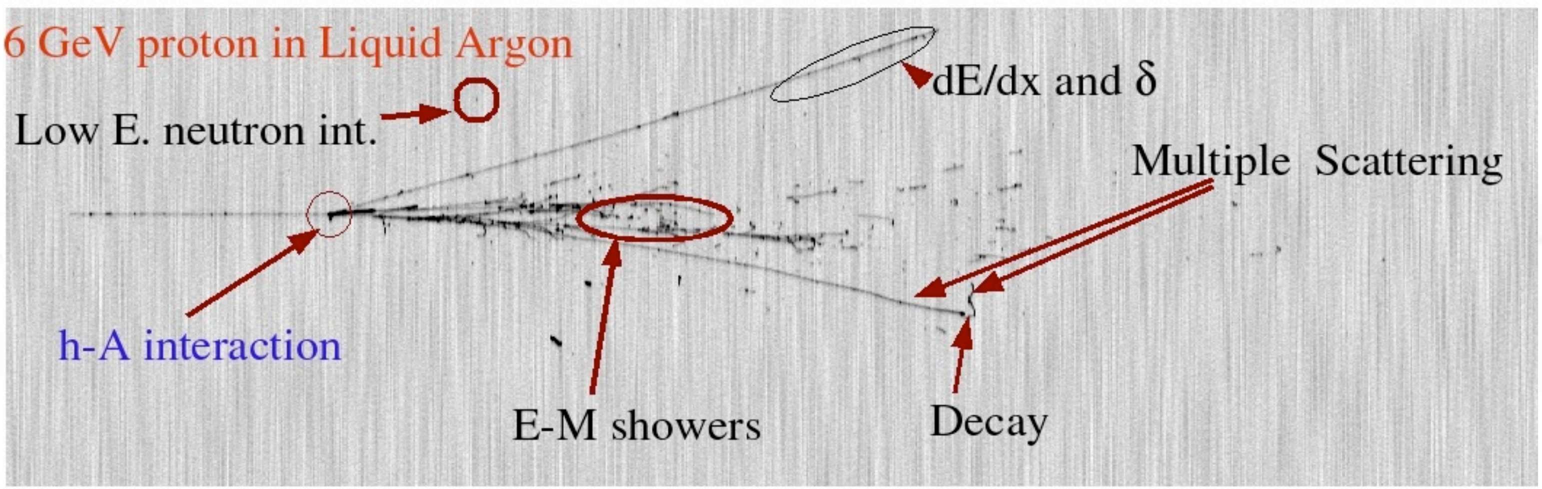
The FLUKA code

http://www.fluka.org

A general purpose tool for calculations of particle transport and interactions with matter: from LHC to microdosimetry

Main authors: A. Fassò, A. Ferrari, J. Ranft, P.R. Sala
Contributing authors: G. Battistoni, F. Cerutti, M. Chin, T. Empl, M.V. Garzelli, M. Lantz, A. Mairani, V. Patera, S. Roesler, G. Smirnov,F. Sommerer, V. Vlachoudis



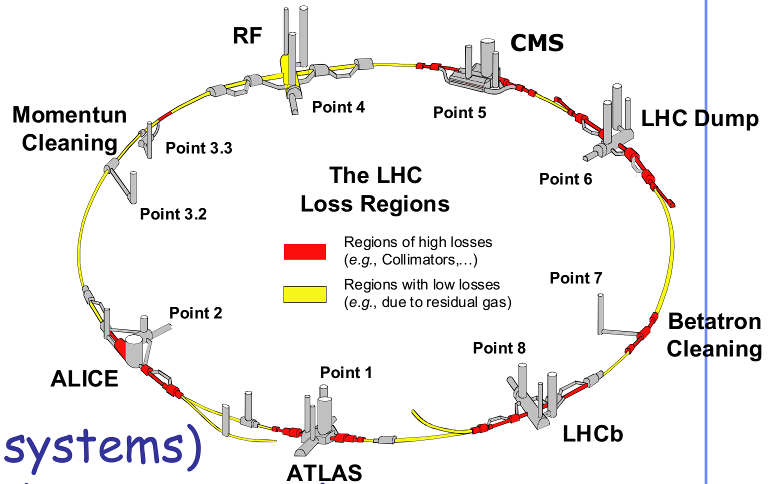
- High accuracy physics models/"microscopic" approach. Benchmarked with exp. data
- Conservation laws implemented at the level of machine accuracy
- Continuous development
- Easy to use for basic applications

FLUKA Description

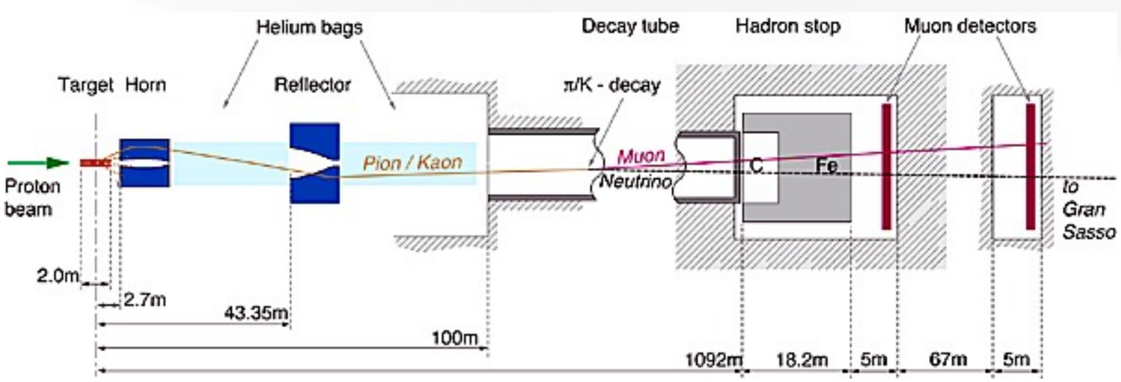
- FLUKA is a general purpose tool for calculations of particle transport and interactions with matter, covering an extended range of applications: from proton and electron accelerator shielding to target design, calorimetry, activation, dosimetry, detector design, Accelerator Driven Systems, cosmic rays, neutrino physics, radiotherapy etc.
- 60 different particles + Heavy Ions
  - Hadron-hadron and hadron-nucleus interaction "0"-10000 TeV
  - Electromagnetic and μ interactions 1 keV – 10000 TeV
  - Nucleus-nucleus interaction up to 10000 TeV/n
  - Charged particle transport and energy loss
  - Neutron multi-group transport and interactions 0-20 MeV
  - n interactions
  - Transport in magnetic field
  - Combinatorial (boolean) and Voxel geometries
  - Double capability to run either fully analogue and/or biased calculations
  - On-line evolution of induced radioactivity and dose
  - User-friendly GUI interface thanks to the Flair interface

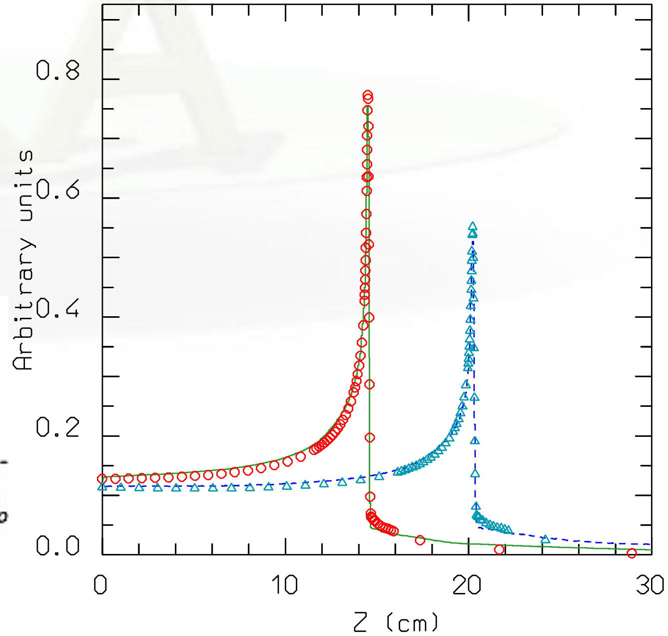
Full mixed field capability

FLUKA Applications



- Cosmic ray physics
- Neutrino physics
- Accelerator design (→ n_ToF, CNGS, LHC systems)
- Particle physics: calorimetry, tracking and detector simulation etc. →ALICE, ICARUS, ...)
- ADS systems, waste transmutation, (→"Energy amplifier", FEAT, TARC,...)
- Shielding design
- Dosimetry and radioprotection
- Space radiation
- Hadrontherapy
- Neutronics





The History

The early days

The beginning:

1962: Johannes Ranft (Leipzig) and Hans Geibel (CERN): Monte Carlo for high-energy proton beams

The name:

1970: study of event-by-event fluctuations in a NaI calorimeter (FLUktuierende KAskade)

Early 70's to ≈1987: J. Ranft and coworkers (Leipzig University) with contributions from Helsinki University of Technology (J. Routti, P. Aarnio) and CERN (G.R. Stevenson, A. Fassò)

Link with EGS4 in 1986, later abandoned

The modern code: some dates

Since 1989: mostly INFN Milan (A. Ferrari, P.R. Sala): little or no remnants of older versions. Link with the past: J. Ranft and A. Fassò

1990: LAHET / MCNPX: high-energy hadronic FLUKA generator *No further update*

1993: G-FLUKA (the FLUKA hadronic package in GEANT3). *No further update*

1998: FLUGG, interface to GEANT4 geometry

2000: grant from NASA to develop heavy ion interactions and transport

2001: the INFN FLUKA Project

2003-2019: CERN-INFN collaboration to develop, maintain and distribute FLUKA

The FLUKA Code design - 1

- Sound and updated physics models
  - Based, as far as possible, on original and well-tested microscopic models
  - Optimized by comparing with experimental data at single interaction level: *"theory driven, benchmarked with data"*
  - Final predictions obtained with minimal free parameters fixed for all energies, targets and projectiles
  - Basic conservation laws fulfilled "a priori"
    - ➔ *Results in complex cases, as well as properties and scaling laws*, arise naturally from the underlying physical models
    - ➔ *Predictivity where no experimental data are directly available*

It is a "condensed history" MC code, with the possibility use of single instead of multiple scattering

The FLUKA Code design - 2

- Self-consistency
  - Full cross-talk between all components: hadronic, electromagnetic, neutrons, muons, heavy ions
  - Effort to achieve the same level of accuracy:
    - for each component
    - for all energies
  - ➔ Correlations preserved fully within interactions and among shower components

Applications in Medical Physics and related disciplines

- Nuclear Medicine
  - Dosimetry
- Radiotherapy
  - Simulation of therapy devices
  - Simulations/Check of treaments
- Hadrontherapy
  - Shielding
  - Commissioning of facilities
  - Treatment planning and forward checks
  - Predictions for monitoring applications (imaging for hadrontherapy)
  - Design of instruments, dosimetry
  - Calculation for shielding and rad. protection in facilities

Using FLUKA

Platform: Linux with g77 (in 32bit mode)
and gfortran (on 64bit machines)

Mac OSX with gfortran

Standard Input:

- Command/options driven by "data cards" (ascii file) .
  Graphical interface is available!!!!

- Standard Geometry ("Combinatorial geometry"): input by "data cards"

Standard Output and Scoring:

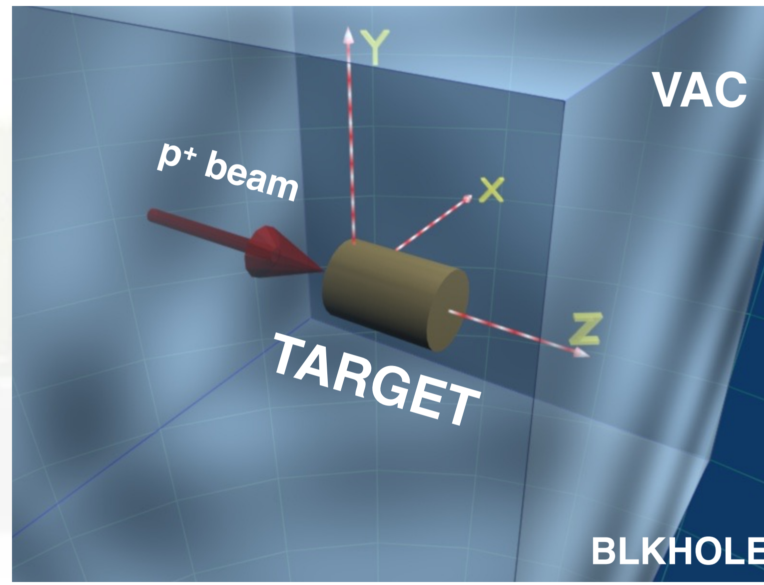
- Apparently limited but highly flexible and powerful
- Output processing and plotting interface available

A Simple Example of basic input

```
TITLE
FLUKA Course Exercise
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....*
DEFAULTS                                                              NEW-DEFA
BEAM             -3.5 -0.082425      -1.7       0.0       0.0       1.0PROTON
BEAMPOS           0.0       0.0       0.1       0.0       0.0       0.0
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....*
GEOBEGIN                                                              COMBNAME
    0    0                  Cylindrical Target
SPH BLK 0.0  0.0  0.0  10000.
* vacuum box
RPP VOI -1000. 1000. -1000. 1000. -1000. 1000.
* Lead target
RCC TARG0.0 0.0 0.0 0.0 0.0 10. 5.
END
* Regions
* Black Hole
BLKHOLE 5    +BLK -VOI
* Void around
VAC     5    +VOI -TARG
* Target
TARGET  5    +TARG
END
GEOEND
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....*
ASSIGNMA    BLCKHOLE   BLKHOLE
ASSIGNMA      VACUUM       VAC
ASSIGNMA        LEAD    TARGET
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....*
RANDOMIZ         1.0
START           10.0       0.0
STOP
```

Primary beam

Geometry



Assignin materials

THE FLUKA COMBINATORIAL GEOMETRY

Introduction

Principle of Combinatorial Geometry: Basic convex shapes (bodies) such as cylinders, spheres, parallelepipeds, etc. are combined to more complex shapes called regions. This combination is done by the boolean operations union, intersection and subtraction.

The Combinatorial Geometry of FLUKA was initially similar to the package developed at ORNL for the neutron and gamma-ray transport program Morse (M.B. Emmett ORNL-4972 1975) which was based on the original combinatorial geometry by MAGI (Mathematical Applications Group, Inc., W. Guber et al, MAGI-6701 1967).

Basic Concepts

Four concepts are fundamental in the FLUKA CG:

- Bodies - basic convex objects, plus infinite planes, infinite cylinders and generic quadric surfaces
- Zones - sub-regions defined only with intersection and subtraction of bodies
- Regions - defined as boolean operations of bodies (union of zones)

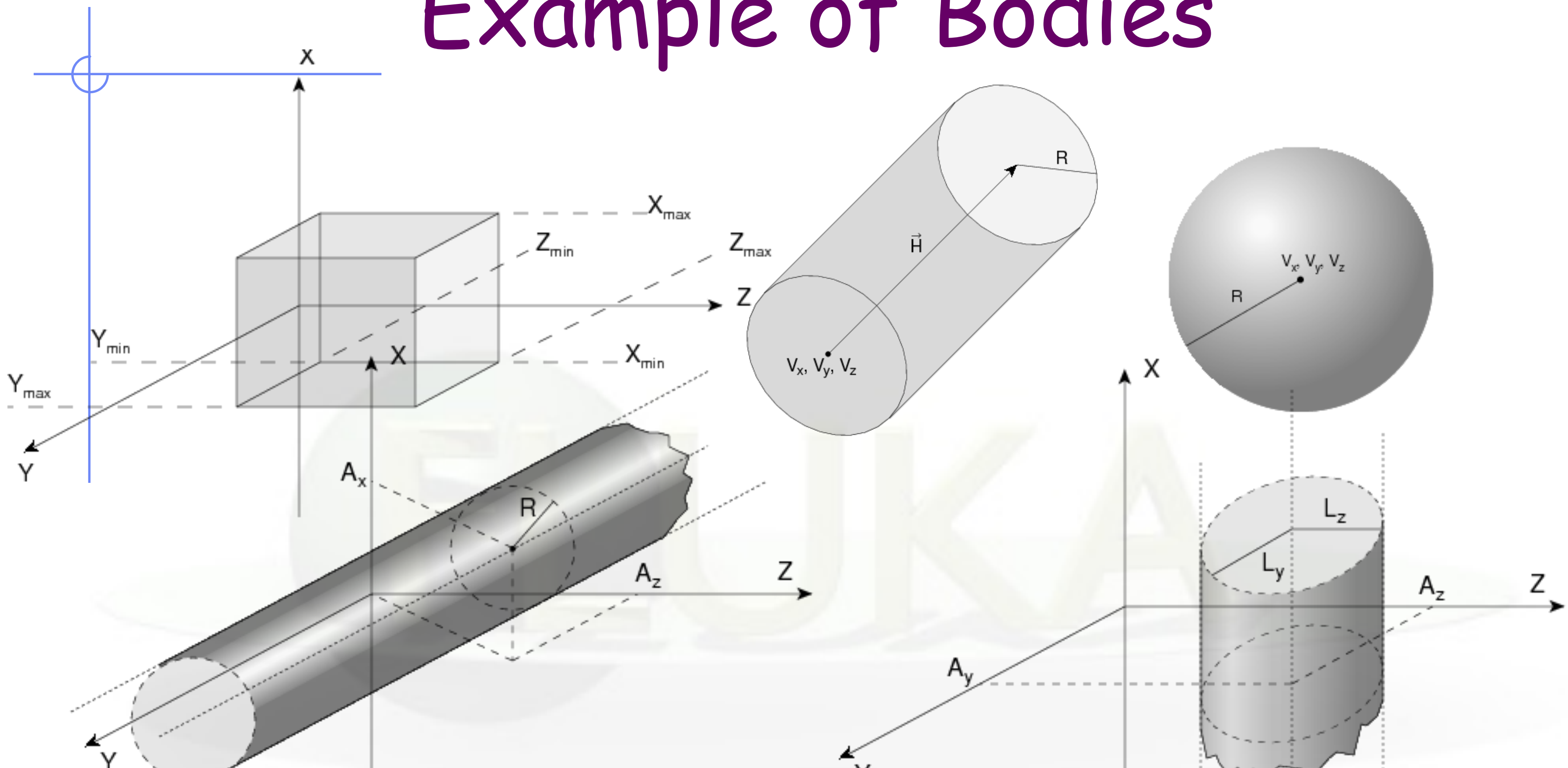
In the original description (Morse) bodies were convex solid bodies (finite portions of space completely delimited by surfaces of first or second degree, i.e. planes or quadrics). In FLUKA, the definition has been extended to include infinite cylinders (circular and elliptical), planes (half-spaces), and generic quadrics (surfaces described by 2nd degree equations)

Use of such "infinite bodies" is encouraged since it makes input less error-prone. They also provide a more accurate and faster tracking.

Bodies

- Each body divides the space into two domains inside and outside. The outside part is pointed to by the normal to the surface.
- 3-character code of available bodies:
  - RPP: Rectangular ParallelePiped
  - SPH: SPHere
  - XYP, XZP, YZP: Infinite half space delimited by a coordinate plane
  - PLA: Generic infinite half-space, delimited by a PLAne
  - XCC, YCC, ZCC: Infinite Circular Cylinder, parallel to coordinate axis
  - XEC, YEC, ZEC: Infinite Elliptical Cylinder, parallel to coordinate axis
  - RCC: Right Circular Cylinder
  - REC: Right Elliptical Cylinder
  - TRC: Truncated Right angle Cone
  - ELL: ELLipsoid of revolution
  - QUA: QUAdric

Example of Bodies



Infinite circular cylinder

Infinite elliptical cylinder

Infinite half-space parallel to coordinate axis

Arbitrarily oriented infinite half-space

Arbitrary generic quadric: corresponding to the equation:

$$A_{xx}\, x^2 + A_{yy}\, y^2 + A_{zz}\, z^2 + A_{xy}\, xy + A_{xz}\, xz + A_{yz}\, yz +$$
$$+ A_x\, x + A_y\, y + A_z\, x + A_0 = 0$$

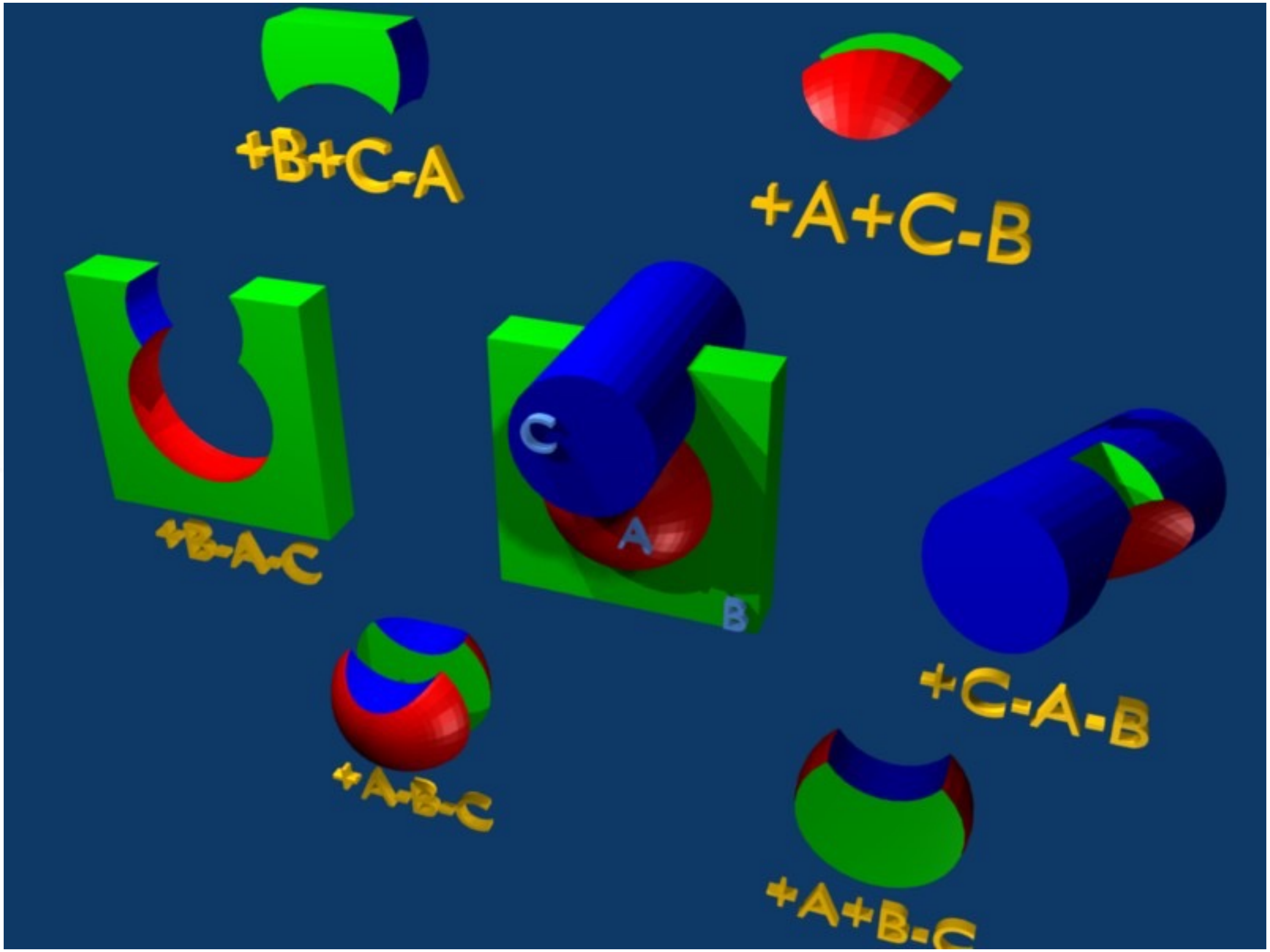
Concept of Region

Regions are defined as combinations of bodies obtained by boolean operations:

	Union	Subtraction	Intersection
Free Format	|	–	+
Fixed format	OR	–	+
Mathematically	∪	−	∩

Regions are not necessarily simply connected (they can be made as the union of two or more non contiguous or partially overlapping zones) but must be of homogeneous material composition.

Illustration of Region building using Boolean operators

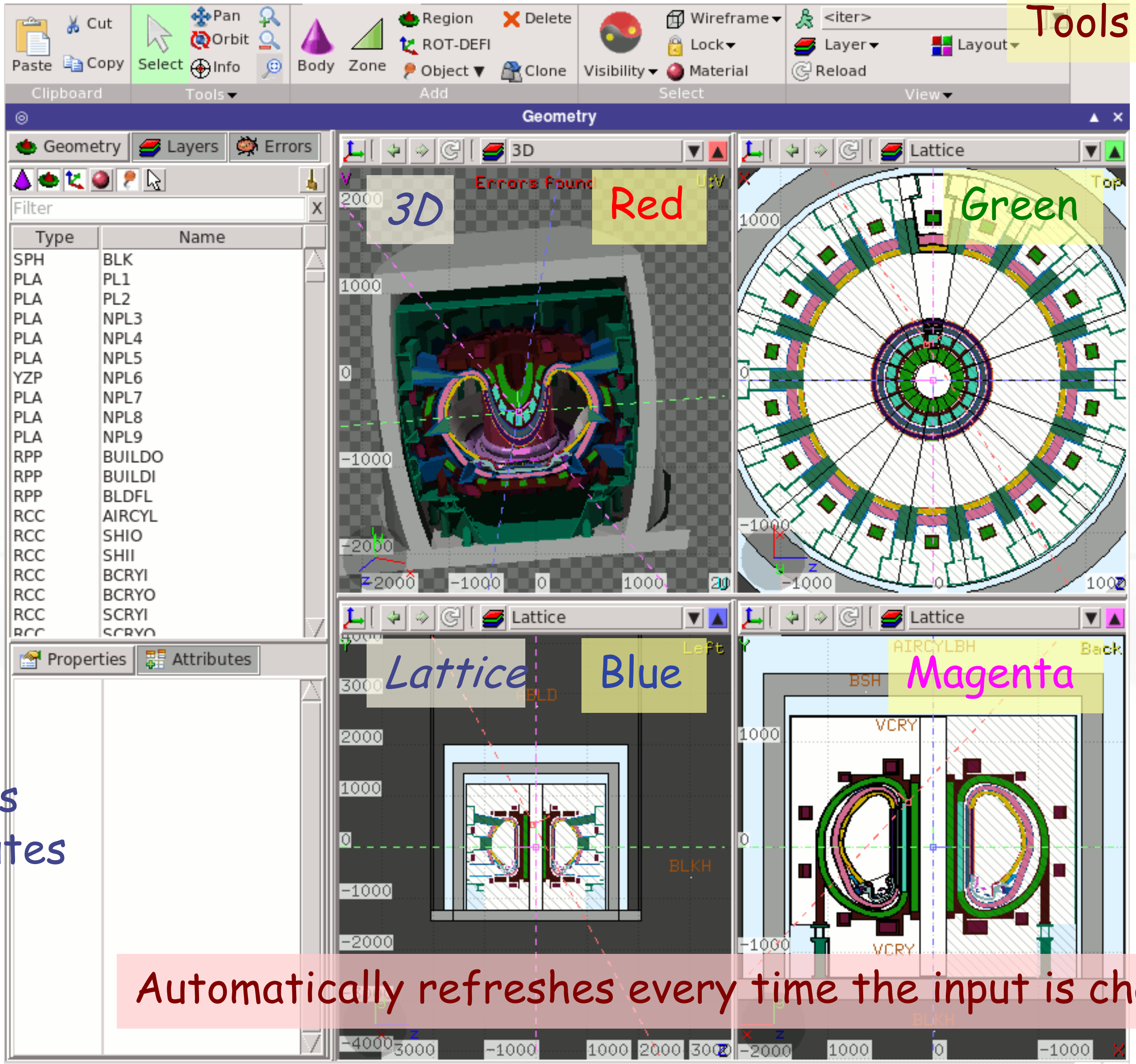


Geometry Editor: Interface

Filter

Filtered Objects

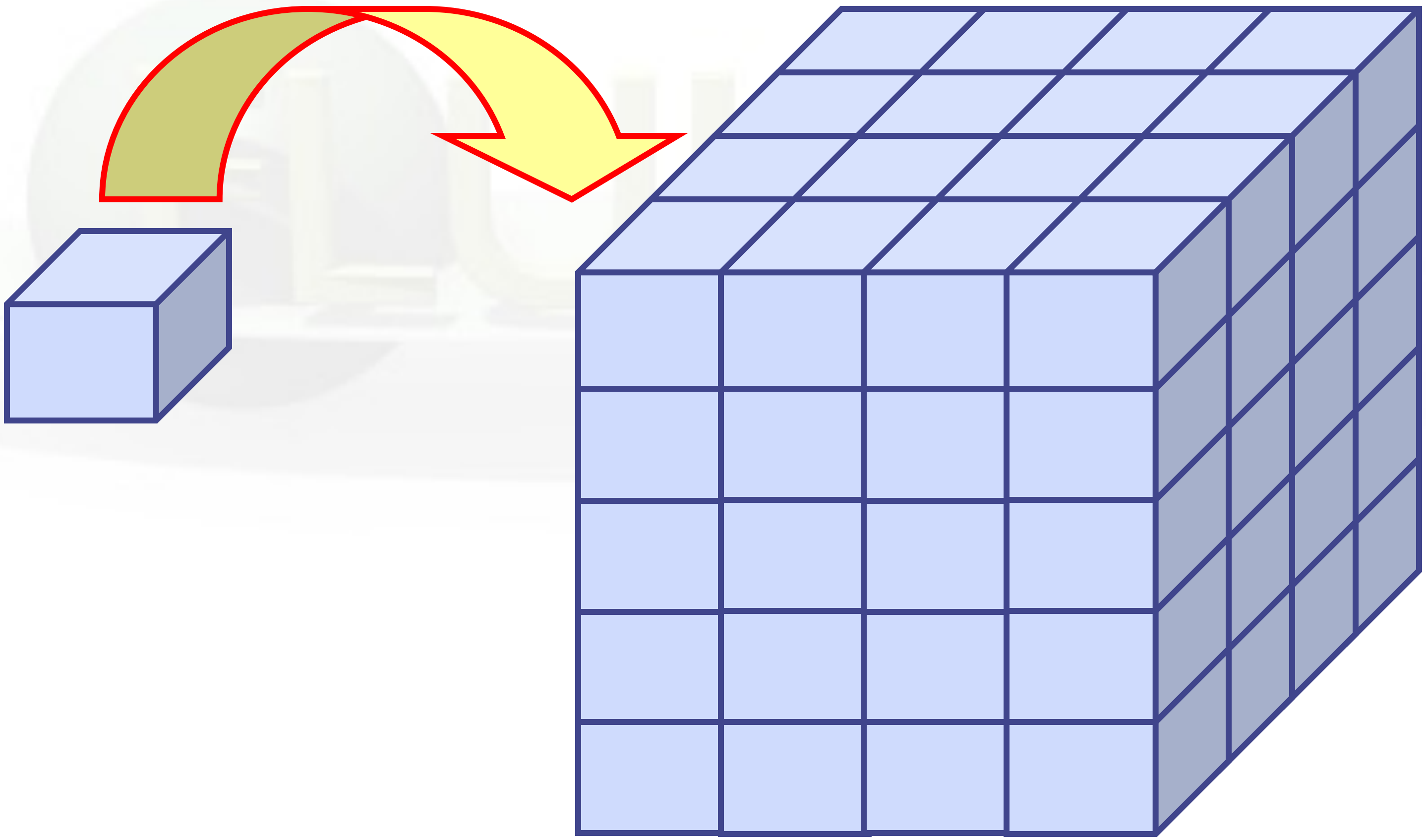
Properties & Attributes



Automatically refreshes every time the input is changed

The FLUKA voxel geometry

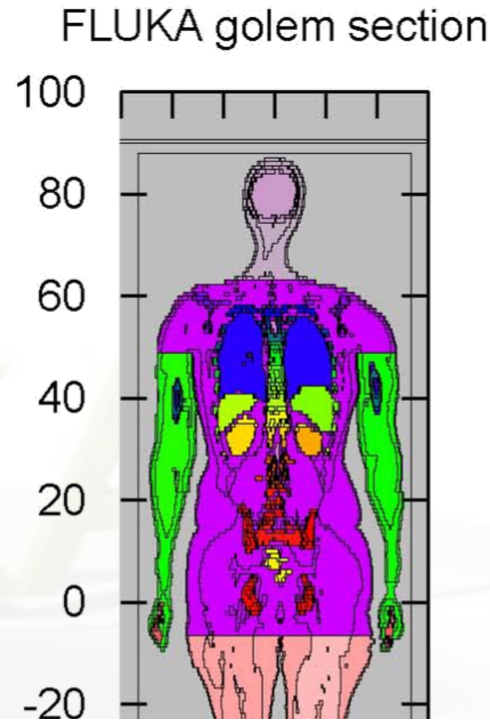
- It is possible to describe a geometry in terms of "voxels", i.e., tiny parallelepipeds (all of equal size) forming a 3-dimensional grid



Voxel geometries: examples

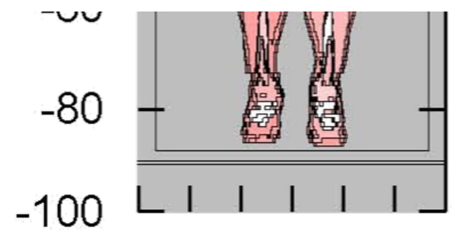
The anthropomorphic
GOLEM phantom

Implementation in FLUKA (radioprotection applications)

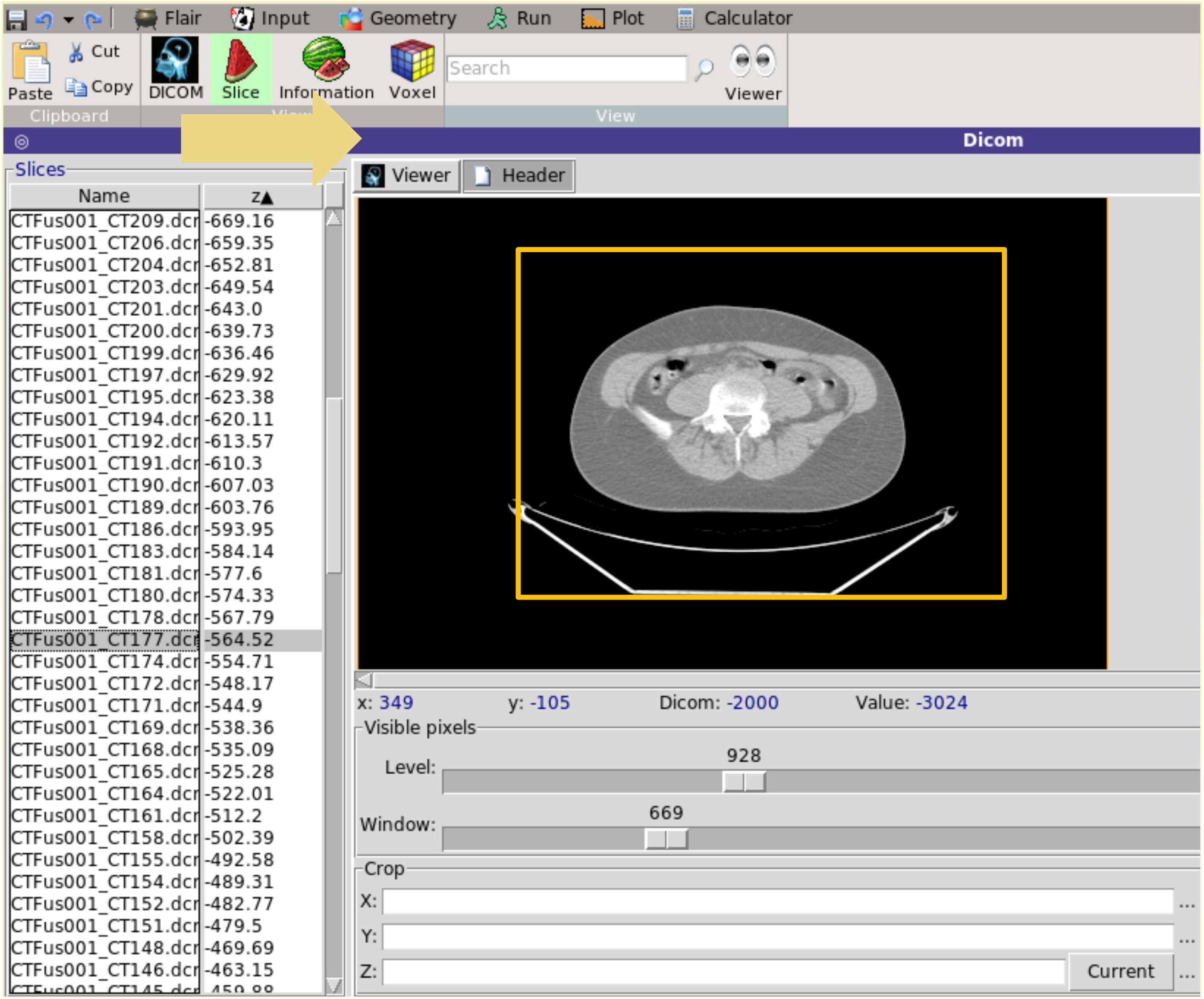


Now available the official ICRP Human Phantom
ICRP Publication 110: Adult Reference Computational Phantoms - *Annals of the ICPR Volume 39 Issue 2*

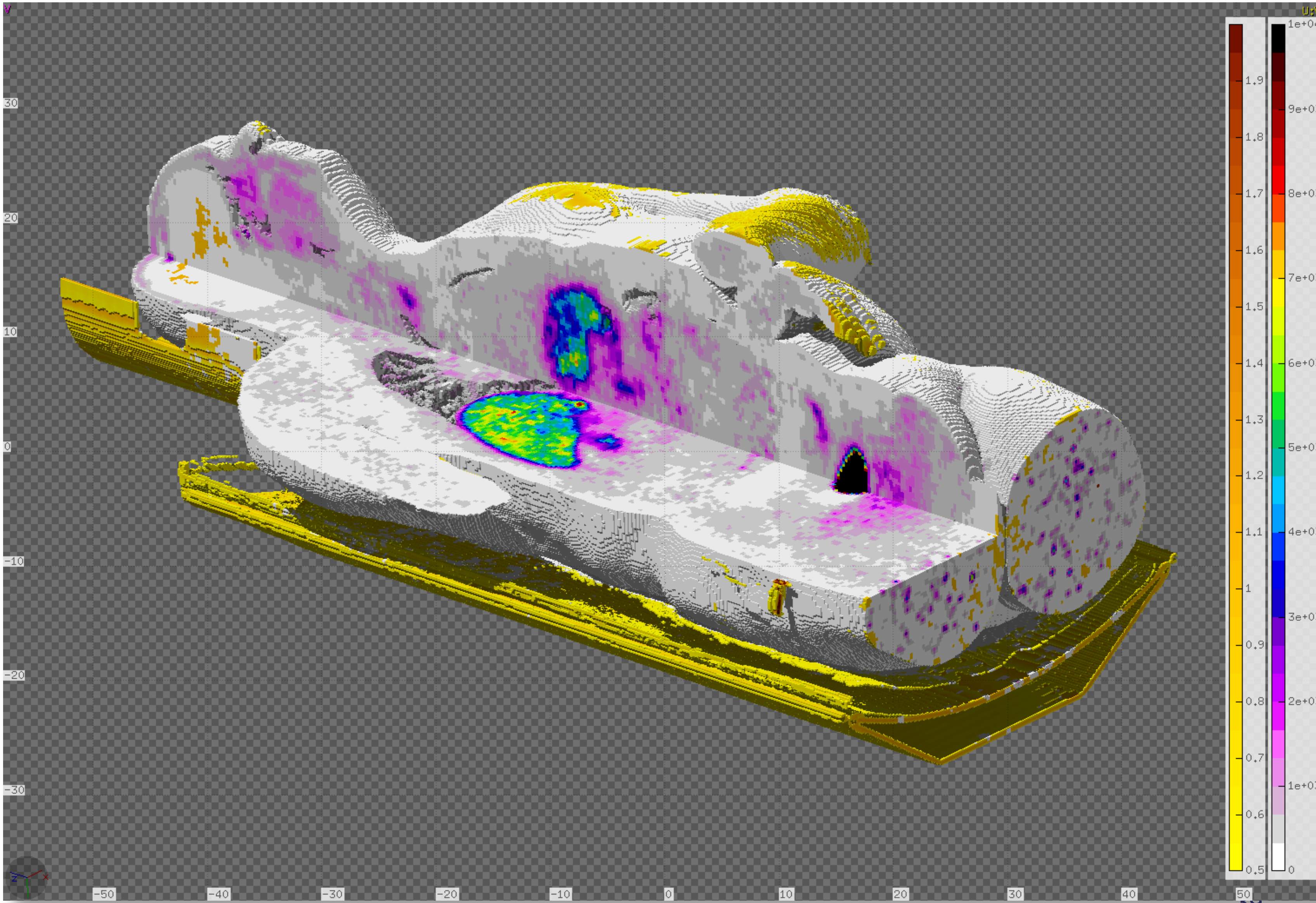
Petoussi-Henss
et al, 2002



Processing the DICOM files the FLUKA graphical interface



Voxel geometry with PET-CT



FLUKA Scoring & Results - Estimators

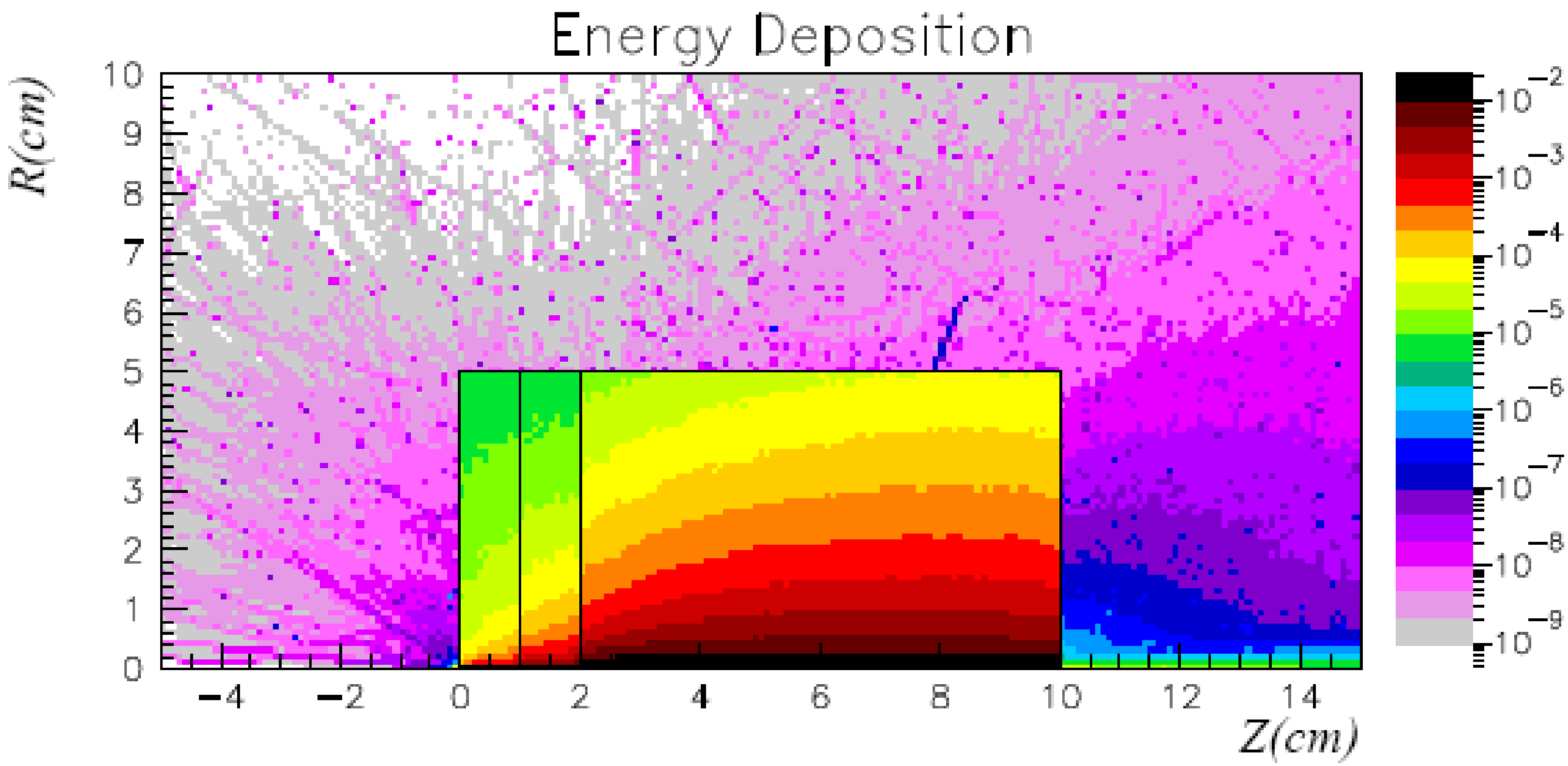
- It is often said that Monte Carlo (MC) is a "mathematical experiment"
  The MC equivalent of the result of a real experiment (*i.e.*, of a measurement) is called an estimator.
- Just as a real measurement, an estimator is obtained by sampling from a statistical distribution and has a statistical error (and in general also a systematic one).
- There are often several different techniques to measure the same physical quantity: in the same way the same quantity can be calculated using different kinds of estimators.
- FLUKA offers numerous different estimators, *i.e.*, directly from the input file the users can request scoring the respective quantities they are interested in.
- As the latter is implemented in a very complete way, users are strongly encouraged to preferably use the built-in estimators with respect to user-defined scoring
- For additional requirements FLUKA user routines are provided

Built-In and User Scoring

- Several pre-defined estimators can be activated in FLUKA.
- One usually refers to these estimators as "scoring" capabilities
- Users have also the possibility to build their own scoring through user routines, HOWEVER:
  - Built-in scoring covers most of the common needs, extensively tested, has refined algorithms for track subdivision, comes with utility programs that allow to evaluate statistical errors takes BIASING weights automatically into account
- Scoring can be geometry dependent AND/OR geometry independent FLUKA can score particle fluences, current, track length, energy spectra, Z spectra, energy deposition...
- Either integrated over the "run", with proper normalization, OR event-by event
- Standard scoring can be weighted by means of simple user routines

USRBIN → The Result

WHAT(2) = ENERGY :Energy deposition from a 3.5 GeV proton beam hitting at [0.,0.,0.] directed along z results are normalized to GeV/cm^3 per primary



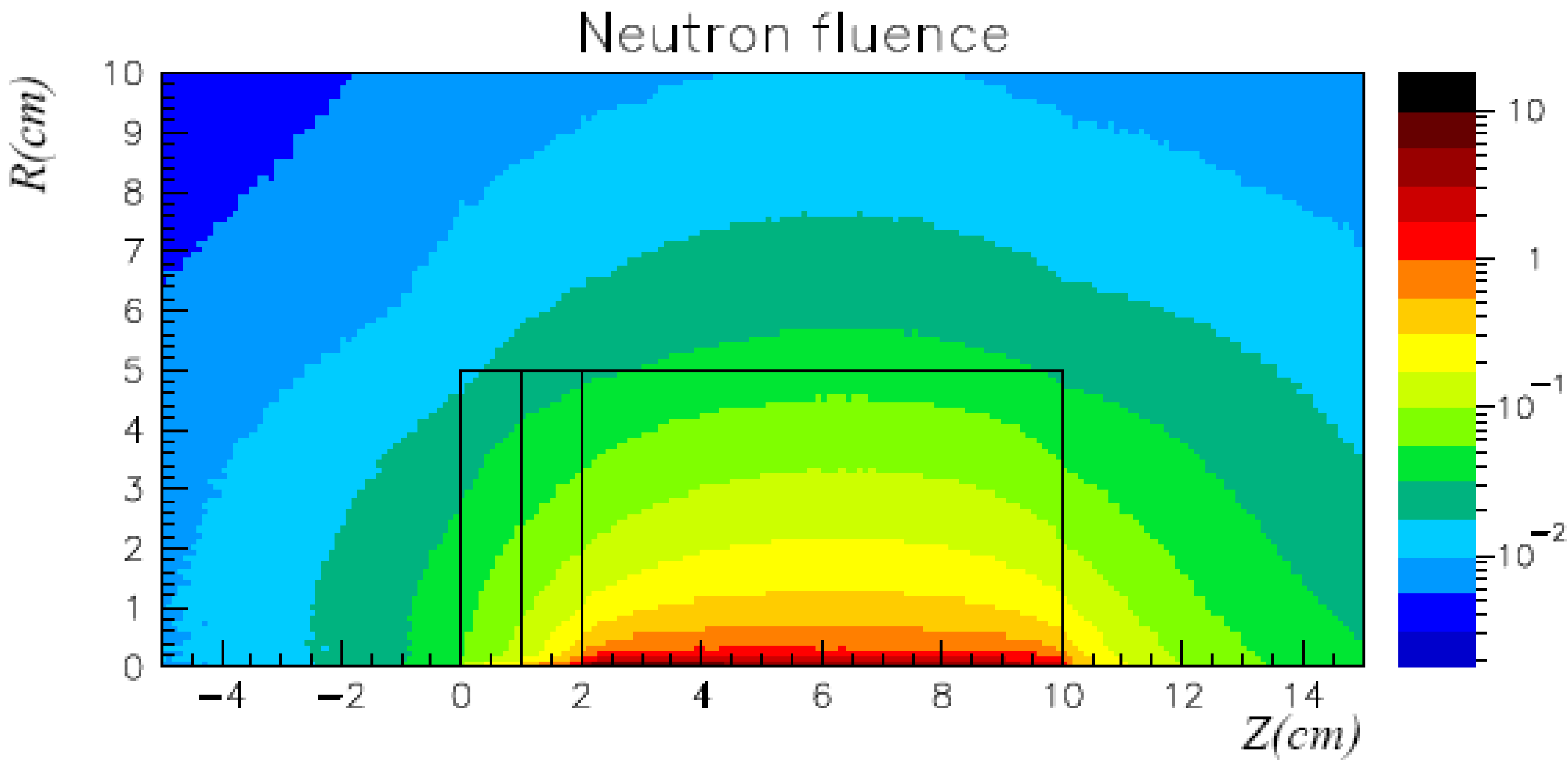
Related Scoring Commands (main cases)

- USRTRACK, USRCOLL score average $d\Phi/dE$ (differential fluence) of a given type or family of particles in a given region
- USRBDX scores average $d^2\Phi/dEd\Omega$ (double-differential fluence or current) of a given type or family of particles on a given surface
- USRBIN scores the spatial distribution of energy deposited, or total fluence (or star density, or momentum transfer) in a regular mesh (cylindrical or Cartesian) described by the user
- USRYIELD scores a double differential yield of particles escaping from a surface. The distribution can be with respect to energy and angle, but also other more "exotic" quantities
- SCORE scores energy deposited (or star density) in all regions

Example of USRBIN → Fluence (1)

Same, WHAT(2)= NEUTRON to get neutron fluence

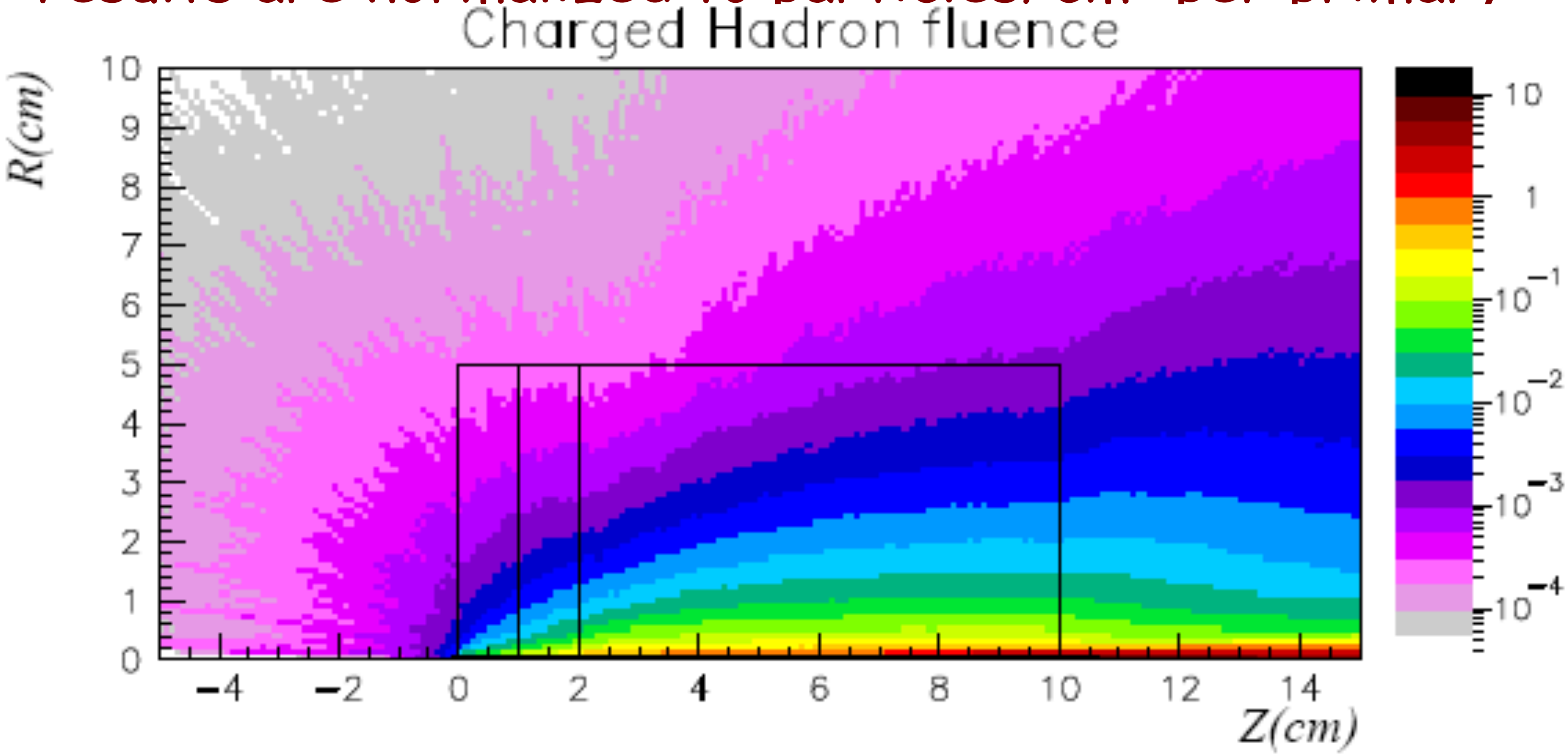
results are normalized to particles/cm^2 per primary



Example of USRBIN → Fluence (2)

Same, WHAT(2)= HAD-CHAR to get charged hadron fluence

results are normalized to particles/cm² per primary



SOMETHING ABOUT THE PHYSICS CONTENT OF FLUKA

E.M. Interactions

- General settings
- Interactions of leptons/photons
  - Photon interactions
    - Photoelectric
    - Compton
    - Rayleigh
    - Pair production
    - Photonuclear
    - Photomuon production
  - Electron/positron interactions
    - Bremsstrahlung
    - Scattering on electrons
  - Muon interactions
    - Bremsstrahlung
    - Pair production
    - Nuclear interactions

- Ionization energy losses
  - Continuous
  - Delta-ray production
- Transport
  - Multiple scattering
  - Single scattering

These are common to all charged particles, although traditionally associated with EM

- Transport in Magnetic field

Ionization energy losses

- Charged hadrons
- Muons
- Electrons/positrons
- Heavy Ions

All share the same approach!

(some extra features are needed for Heavy Ions)

Atomic energy losses:
Bethe-Bloch + higher order (Z^3, Z^4, Mott) corrections

Besides Coulomb scattering with atomic electrons, particles undergo Coulomb scattering also with atomic nuclei

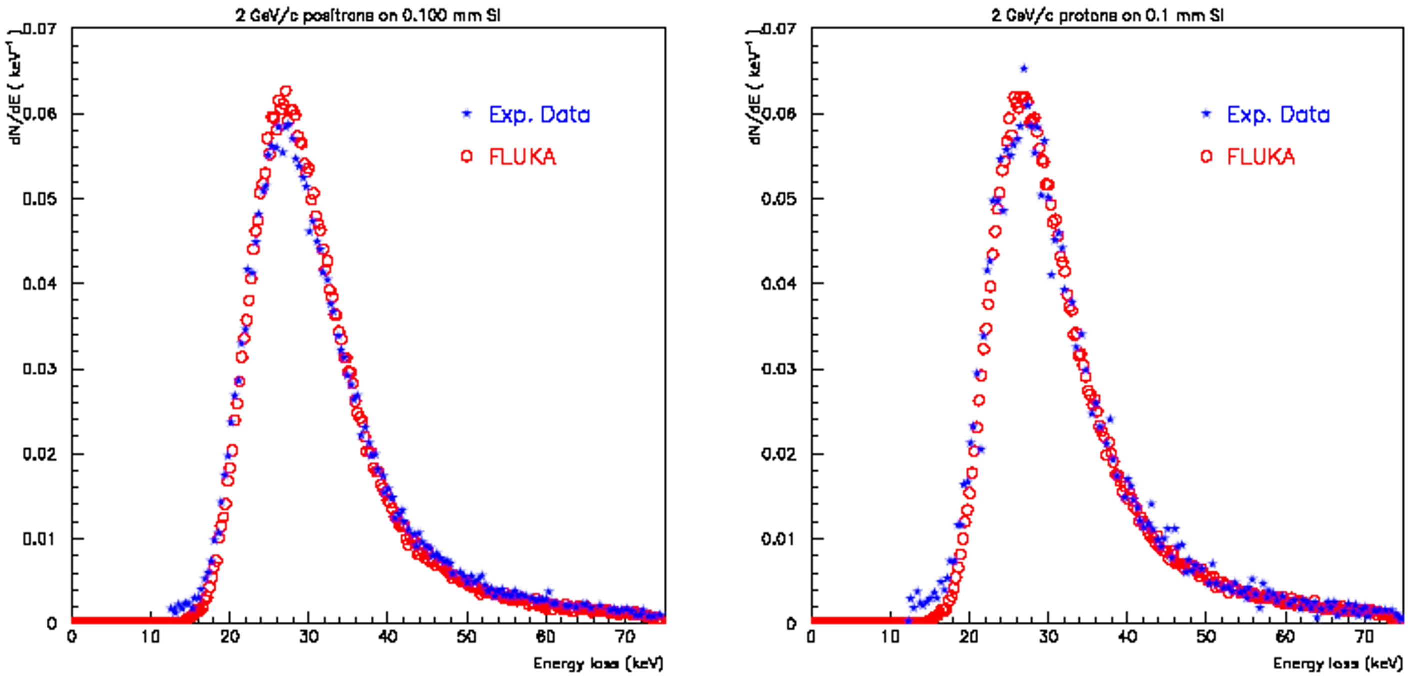
The resulting energy losses, called nuclear stopping power, are smaller than the atomic ones, but are important for heavy particles

Discrete and continuous energy loss

- Discrete energy loss (above the δ-ray production threshold)
  - Represents the energy loss of a charged particle due to the explicit production of a δ-ray at the end of a step
  - The cross section for generating a δ-ray is evidently driven by the production threshold (set by the user!)
  - δ-rays can transport energy away from their point of origin
- Continuous energy loss (below the δ-ray production threshold)
  - The cumulative effect of ionization and excitation events below the production threshold is accounted for as continuous energy loss along a particle step
  - The energy deposition due to the continuous energy loss of charged particles is local (i.e. energy not carried away by secondary particles

Ionization fluctuations

FLUKA has a specific model which overcomes the limitations existing for Landau and Vavilov distributions



Experimental [1] and calculated energy loss distributions for 2 GeV/c positrons (left) and protons (right) traversing 100µm of Si

J.Bak et al. NPB288, 681 (1987)

Transport thresholds

In a MC simulation particles are not tracked until they "have lost all their kinetic energy", but until their energy drops to/below a preset transport threshold

When a particle's energy drops below threshold, what happens?

In FLUKA energy is depositedon the spot(for electrons) or ranged out (for heavier projectiles).

General guidelines to set threshold energies?

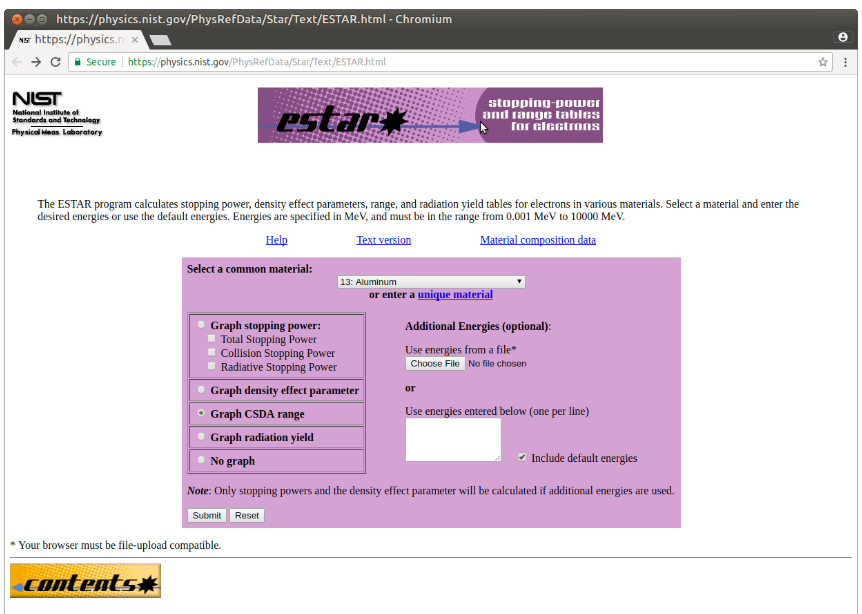
It depends on the "granularity" of the geometry and/or of the scoring mesh. Energy/range tables are very useful.
- Consider the interest in a given region.
- Warning 1: to reproduce correctly electronic equilibrium, neighboring regions should have the same electron energy(NOT range) threshold. To be kept in mind for sampling calorimeters
- Warning 2: Photon thresholds should be lower than electron thresholds (photons travel farther)
- Warning 3: **low thresholds for e-/e+/gammas are CPU eaters**

Transport thresholds - 2

Delta-ray production threshold:
- If production threshold < transport threshold: CPU wasted in producing and dumping particles on the spot
- If production threshold > transport threshold: the latter is increased.

Examine the particle's range

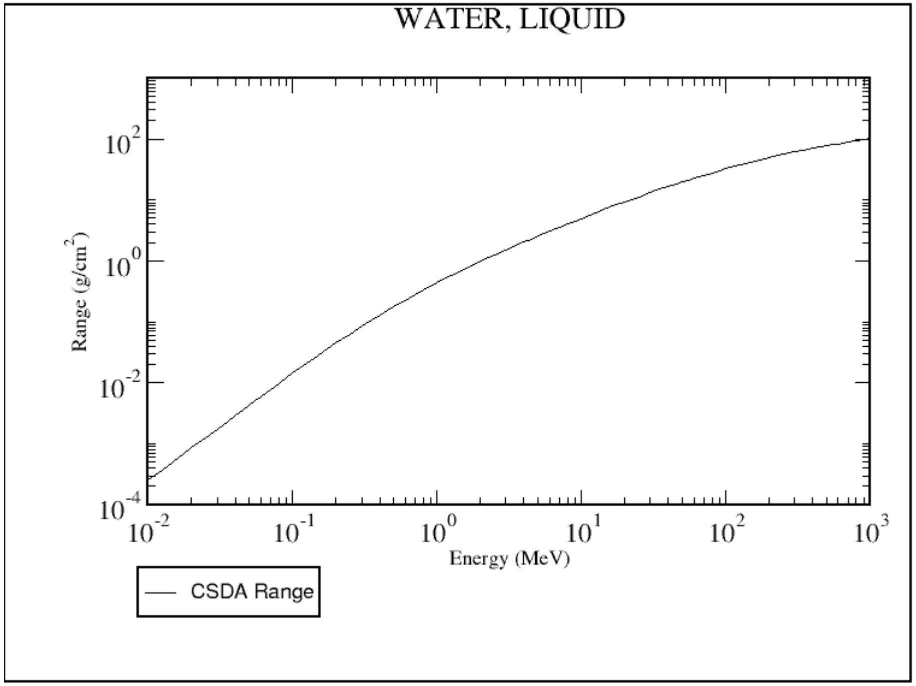
https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html



Transport thresholds - 3

Range for electrons in water

Water density: 1 g/cm^3 → We may directly read range in cm



Transport threshold at 1 MeV? → 1-MeV e^- range is O(1 mm) = 1000 μm
Depositing/killing them on the spot in a ~50 μm geometry is asking too much...

Transport threshold at 10 keV? →10-keV e^- range is O(10^{-4}) cm = O(1 μm)
Depositing them on the spot in a ~50 μm geometry is fine

Charged particle transport

Besides energy losses, charged particles undergo scattering by atomic nuclei. The Molière multiple scattering (MCS) theory is used with the inclusions of corrections to take into account the following items:

- Final deflection wrt initial direction
- Lateral displacement during the step
- Shortening of the straight step with respect to the total trajectory due to “wiggliness” of the path (often referred to as PLC, path length correction)
- Truncation of the step on boundaries
- Interplay with magnetic field

⇒ On user request, a full Single Scattering option is also available: to be used for very thin layers, wires, or gases, where Molière theory does not apply.

The FLUKA hadronic Models

Hadron-nucleus: PEANUT

Elastic, exchange
Phase shifts
data, eikonal

P<3-5GeV/c
Resonance prod
and decay

low E
π, K
Special

High Energy
DPM
hadronization

Sophisticated
G-Intranuclear Cascade

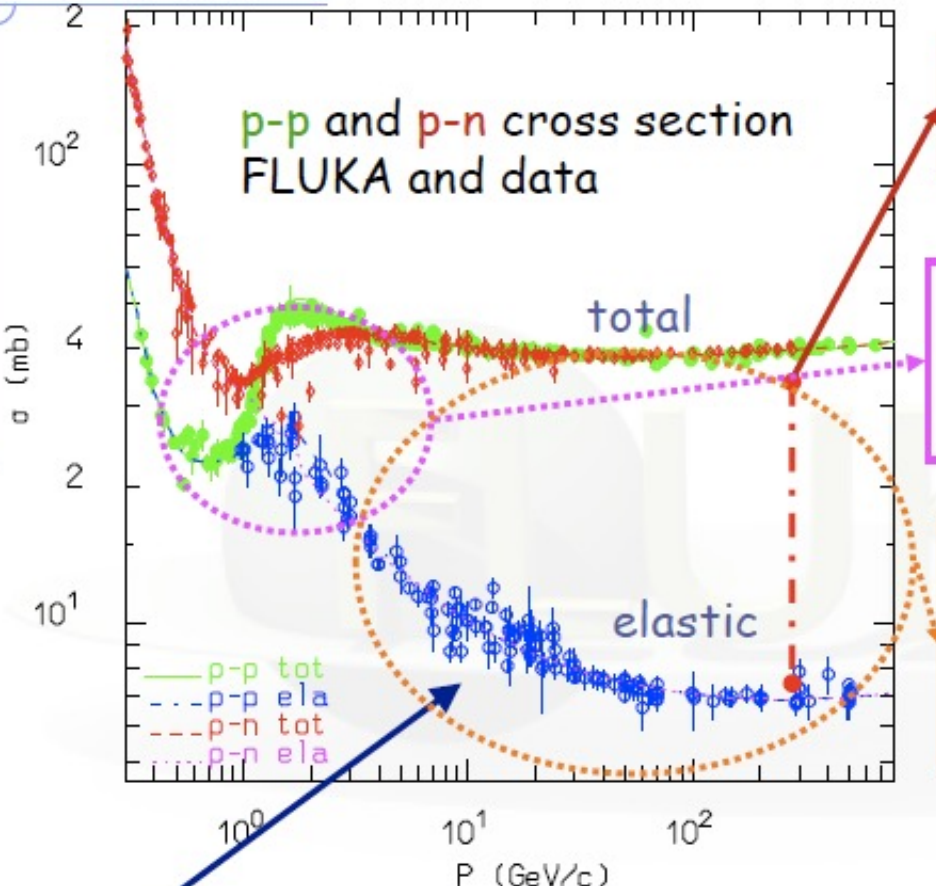
Gradual onset of
Glauber-Gribov multiple
interactions

Preequilibrium

Coalescence

Evaporation/Fission/Fermi break-up
γ deexcitation

Hadron-nucleon interaction models



Particle production interactions: two kinds of models

Those based on "resonance" production and decays, cover the energy range up to 3-5 GeV

Those based on quark/parton string models, which provide reliable results up to several tens of TeV

Elastic, charge exchange and strangeness exchange reactions:

- Available phase-shift analysis and/or fits of experimental differential data
- At high energies, standard eikonal approximations are used

Heavy ion interaction models in FLUKA - 1

The choice of the model is automatic. The user is not requested to provide specifications

E > 5 GeV/n

Dual Parton Model (DPM)

DPMJET-III (original code by R.Engel, J.Ranft and S.Roesler, FLUKA-implemenation by T.Empl *et al.*)

0.1 GeV/n < E < 5 GeV/n

Relativistic Quantum Molecular Dynamics Model (RQMD)

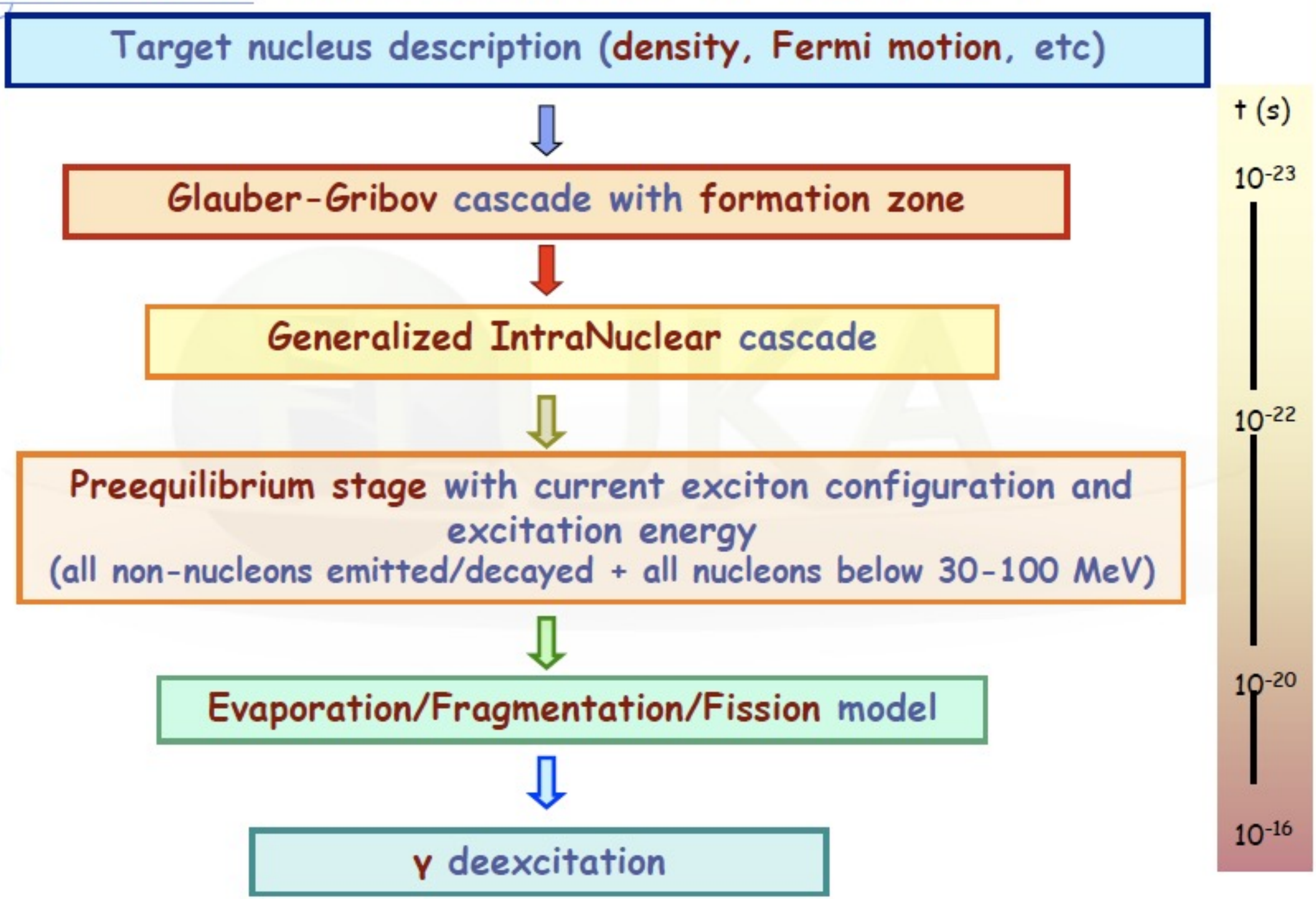
RQMD-2.4 (original code by H.Sorge *et al.*, FLUKA-implementation by A.Ferrari *et al.*)

E < 0.1 GeV/n

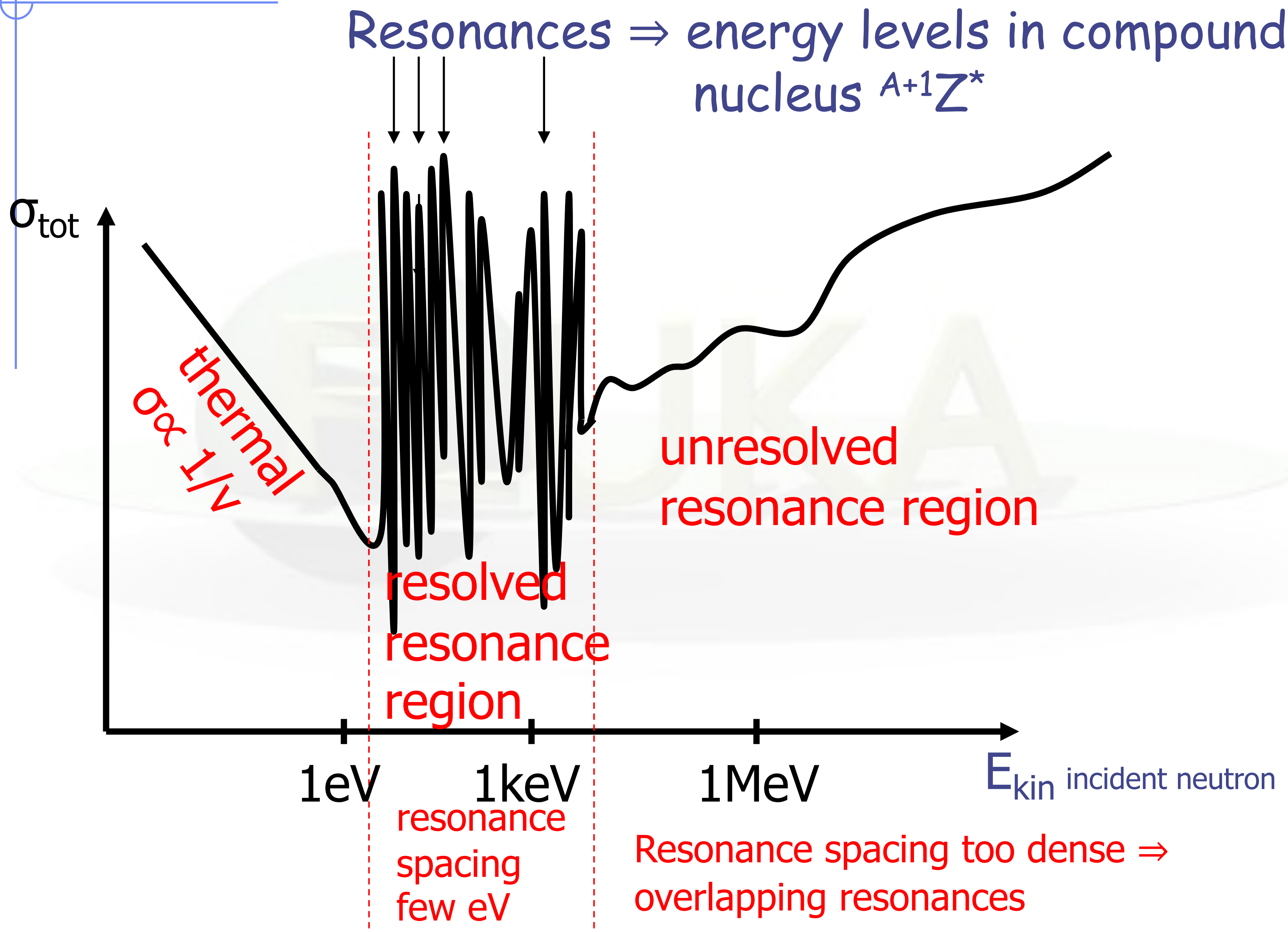
Boltzmann Master Equation (BME) theory

BME (original code by E.Gadioli *et al.*, FLUKA-implementation by F.Cerutti *et al.*)

Nuclear Interactions



Typical neutron cross section



Evaluated Nuclear Data Files

- Evaluated nuclear data files (ENDF, JEFF, JENDL...)
  - typically provide neutron σ (cross sections) for E<20MeV for all channels
  - σ are stored as continuum + resonance parameters
  - Complex programs like NJOY, PREPRO convert the ENDF file to P-ENDF (point-wise cross sections), or G-ENDF (group-wise) including Doppler broadening etc.

Point-wise and Group-wise cross sections

- In neutron transport codes in general two approaches used: point-wise ("continuous" cross sections) and group-wise transport
- Point-wise follows cross section precisely but is can be time and memory consuming
- Group approach is widely used in neutron transport codes because it is fast and gives good results for most applications

Group Transport Technique

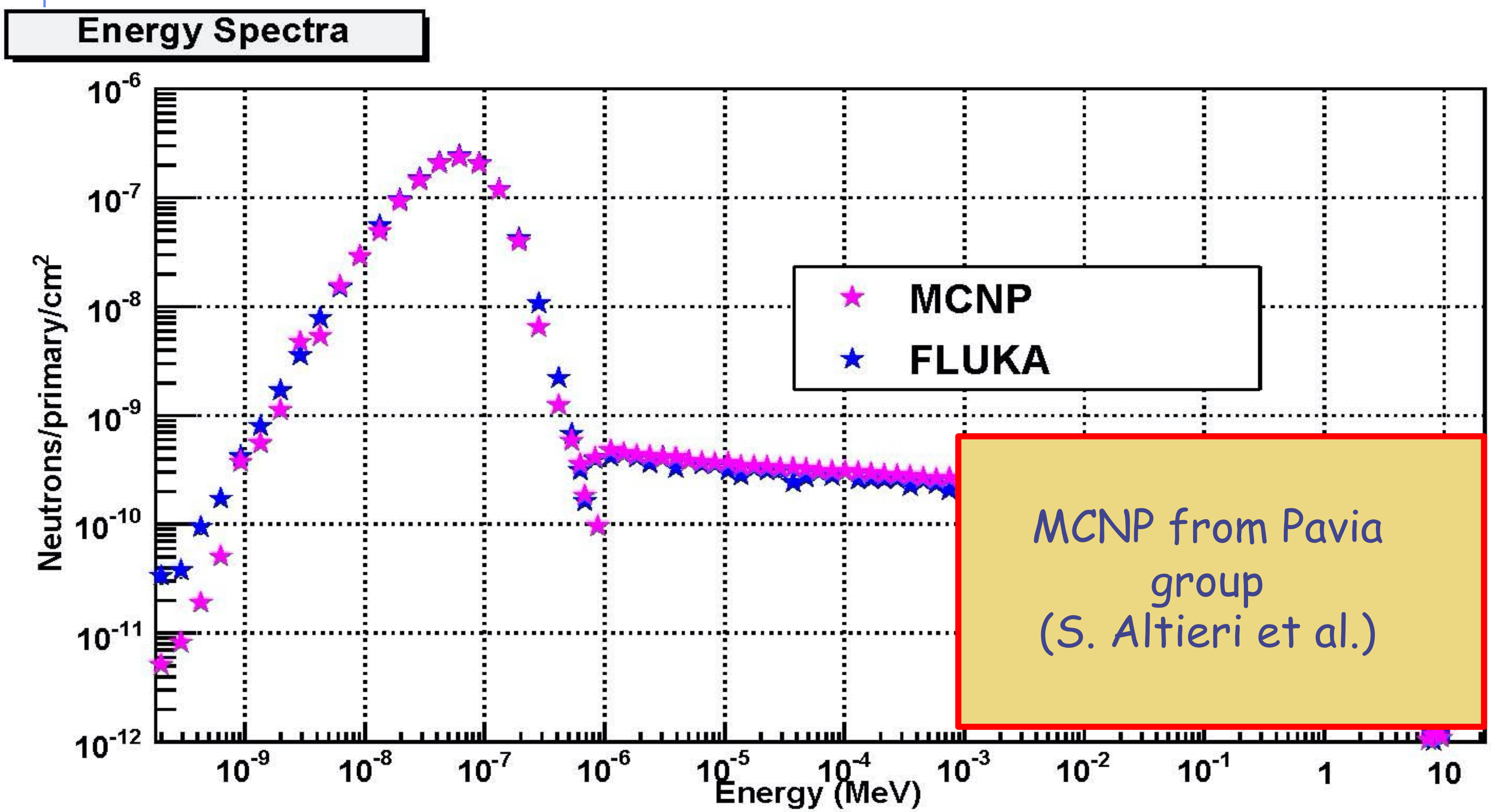
- The energy range of interest is divided in a given number of discrete intervals ("energy groups")
- Elastic and inelastic reactions simulated not as exclusive processes, but by group-to-group transfer probabilities (downscattering matrix)
- Downscattering matrix: if a neutron in a given group undergoes a scattering event and loses energy, it will be transferred to a group of lower energy (each of the lower energy groups having a different probability)
- If the neutron does not lose enough energy to be in another group, it will stay in the same group (in-scattering).
- In thermal region neutrons can gain energy. This is taken into account by an upscattering matrix, containing the transfer probability to a group of higher energy

The FLUKA Low Energy (<20 MeV) Neutron Library

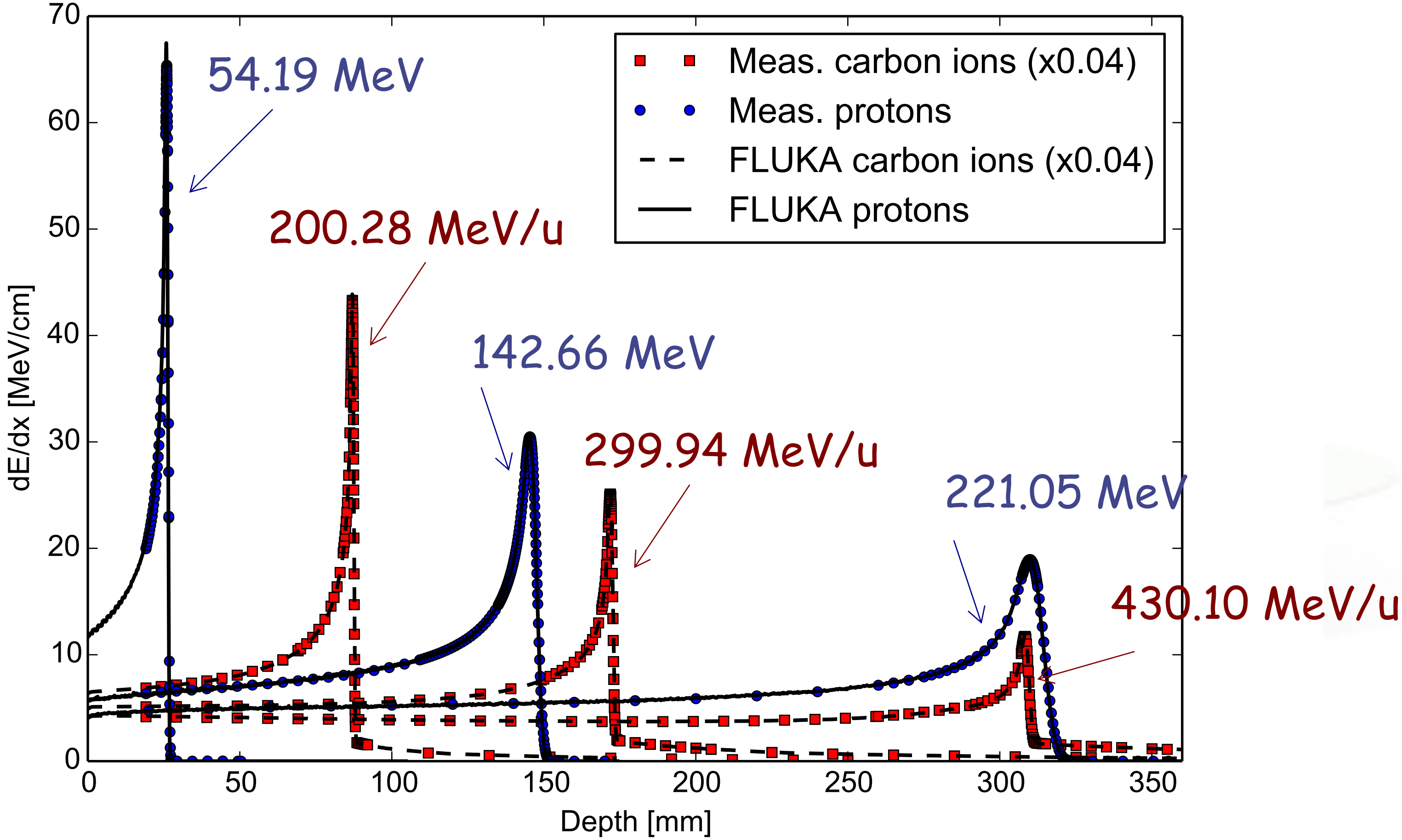
- FLUKA uses the multigroup transport technique
- The energy boundary below which multigroup transport takes over depends in principle on the cross section library used. In the present library it is 20 MeV.
- Both fully biased and semi-analog approaches are available
- Number of groups: 260 of approximately equal logarithmic with, the actual energies limits of each group can be found in the manual (or can be printed to *.out file)
- N.B. the group with the highest energy has the number 1, the group with the lowest energy has number 260
- 31 thermal groups, with 30 upscattering groups
- Energy range of library: 0.01 meV - 20 MeV

⇒ The most recent FLUKA versions has now the possibility of using PointWise neutron cross sections also for E<20 MeV

Simulation of neutron spectrum from reactor (Pavia)

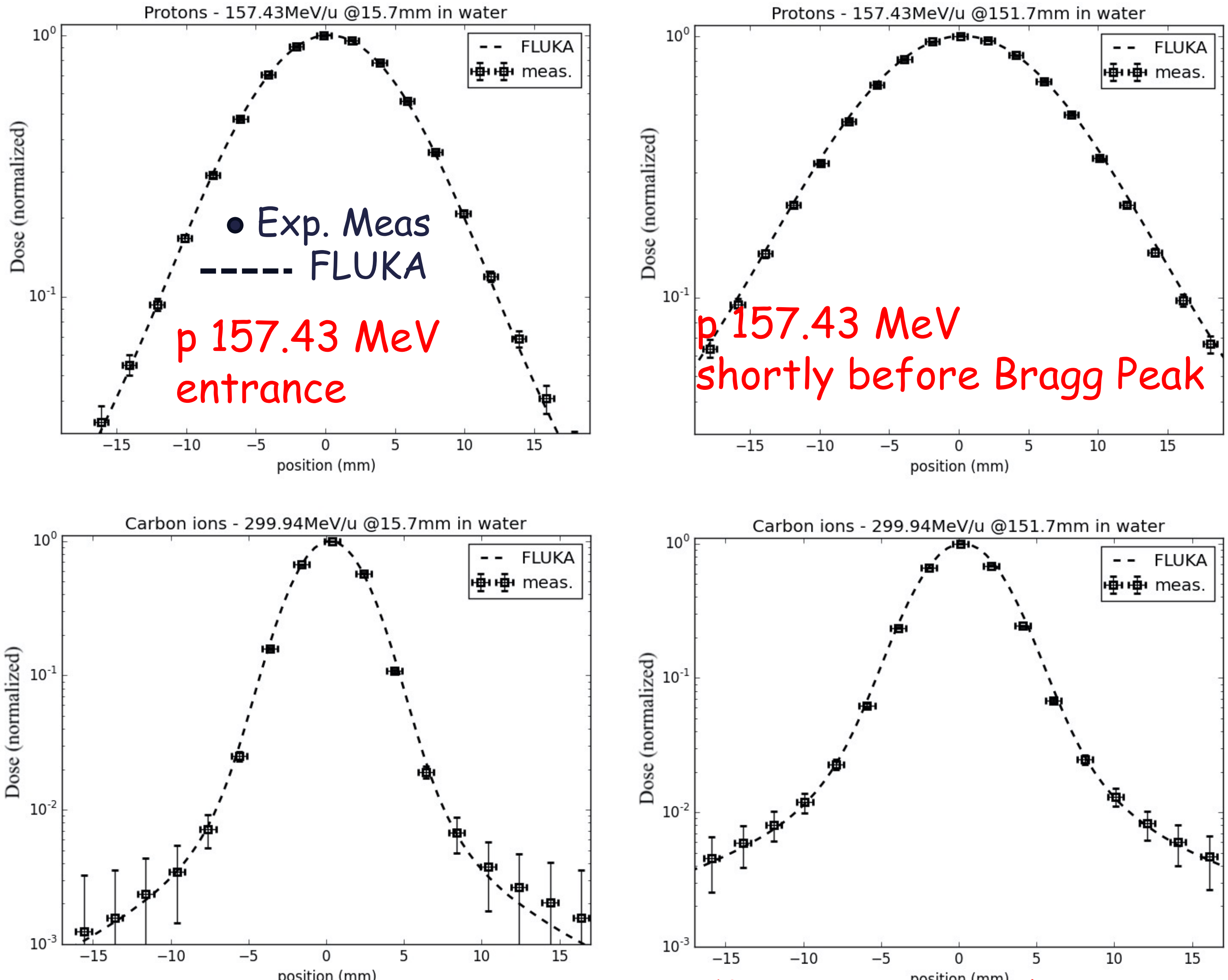


Comparing Predictions for Depth-Dose curves and Lateral Dose Profiles



FlUKA simulations of depth-dose profiles of protons and carbon ions with therapeutic ranges in comparison with measured data at HIT.

Lateral profiles measured @HIT

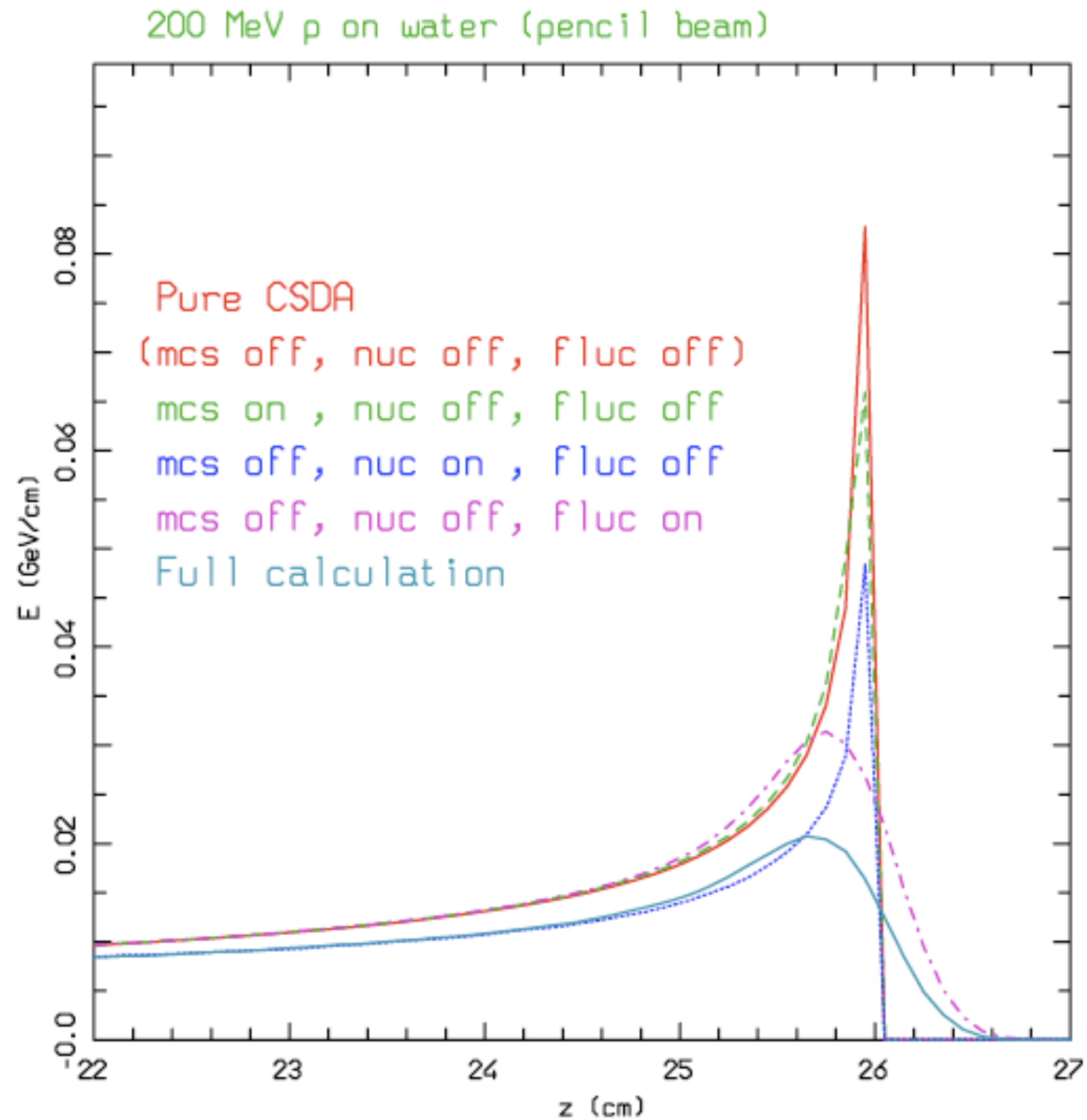


^{12}C 299.94 MeV/u
entrance

^{12}C 299.94 MeV/u
shortly before Bragg Peak

Playing with a proton beam

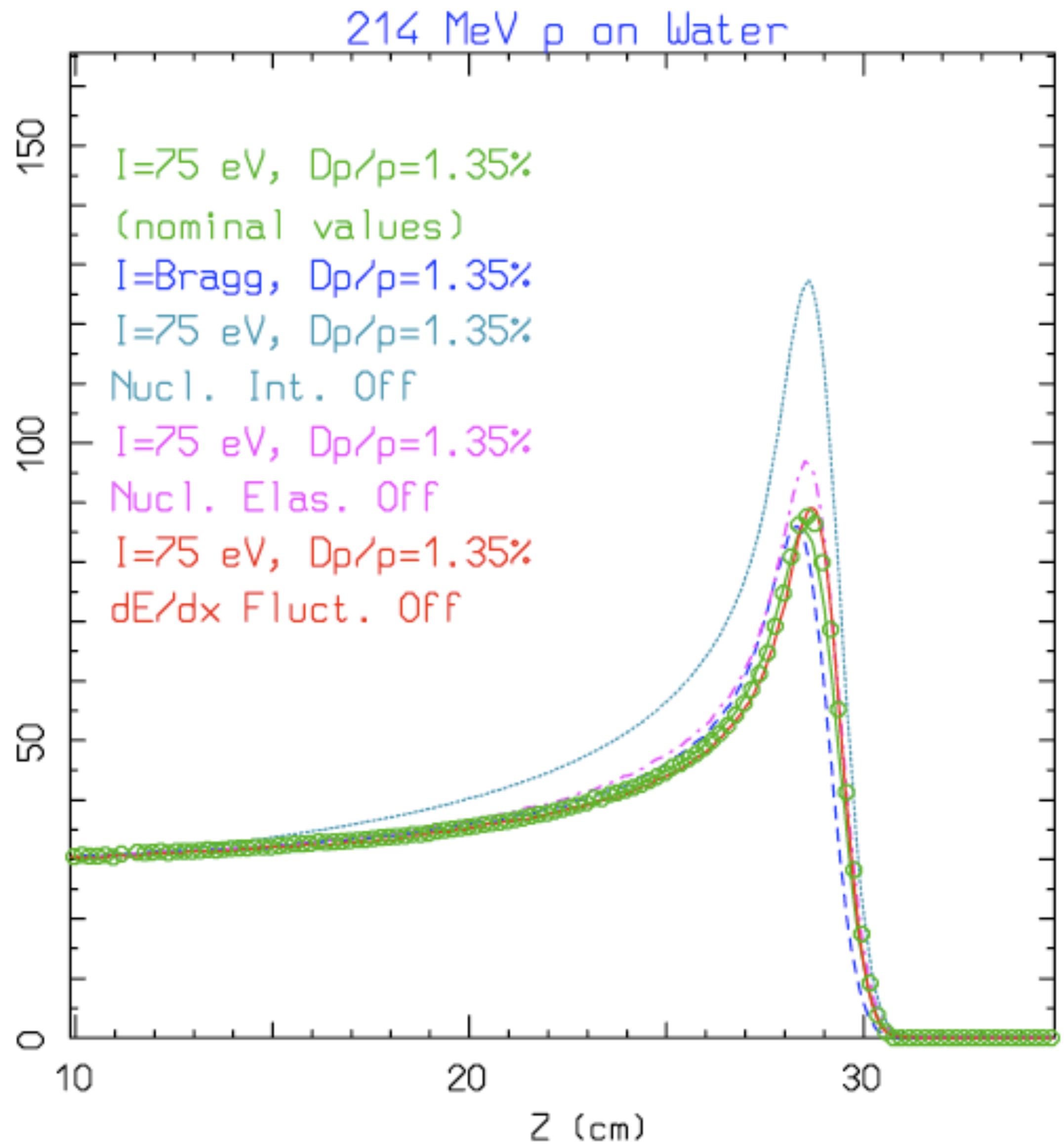
Dose vs depth energy deposition in water for a 200 MeV p beam with various approximations for the physical processes taken into account



Playing with a proton beam II part

Dose vs depth energy deposition in water for a 214 MeV real p beam under various conditions.

Exp. Data from PSI

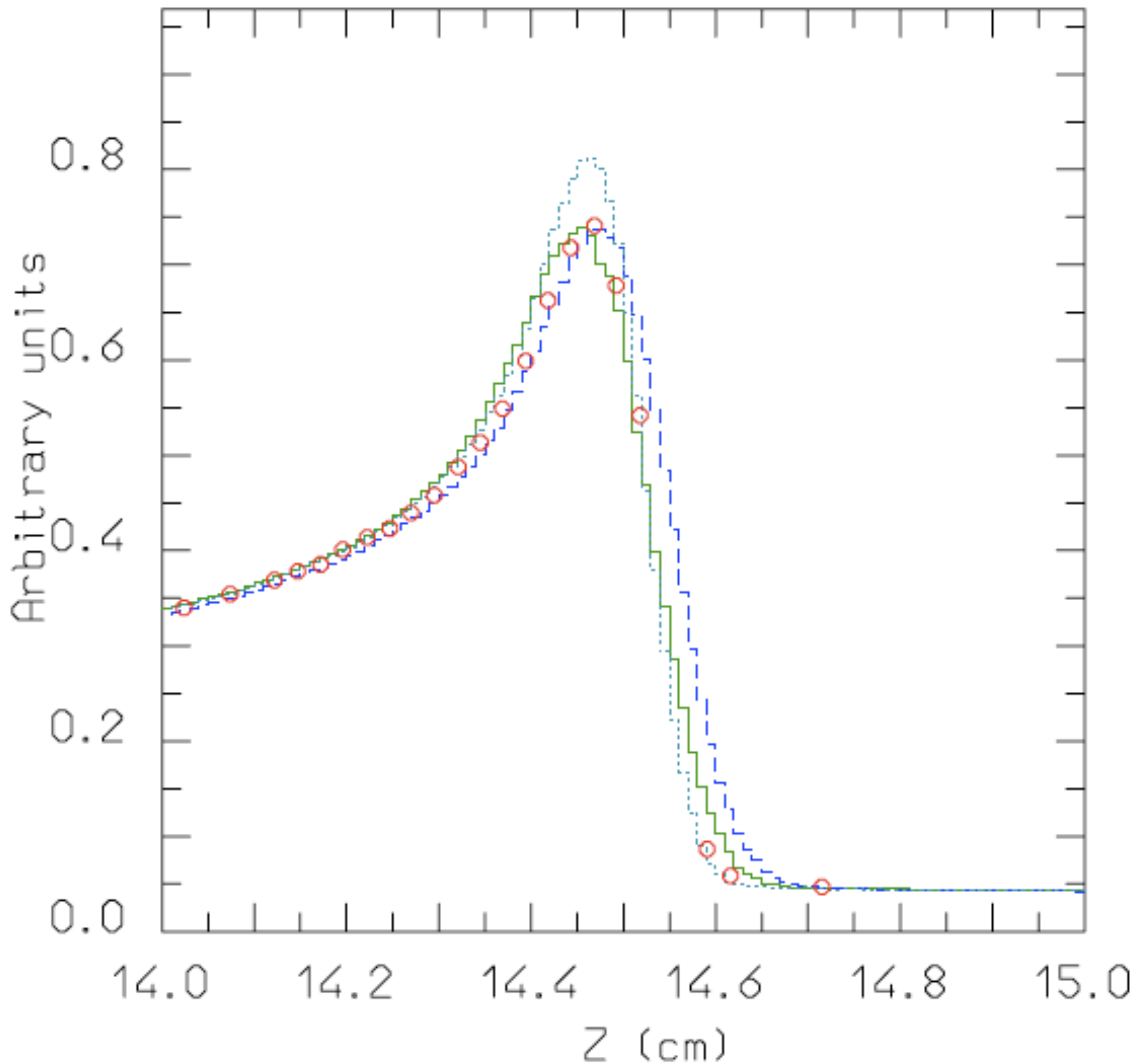


Bragg peaks vs exp. data: ^{12}C @ 270 MeV/n

Close-up of the dose vs depth distribution for 270 MeV/n ^{12}C ions on a water phantom.

The green line is the FLUKA prediction with the nominal 0.15% energy spread

The dotted light blue line is the prediction for no spread, and the dashed blue one the prediction for *I* increased by 1 eV



Exp. Data Jpn.J.Med.Phys. 18, 1,1998

New Technological Developments for Fast Calculations: the GPU MC – 1`

The progress in the use of graphics processing units (GPU) allowed for the development of techniques for general purpose computing exploiting the high degree of parallel operation which characterize these hardware units.
This has brought to the approach denominated "General Purpose computing with Graphics Processing Units" (GPGPU) which includes MC code and their application in medicine, mostly for dose calculations.

High degree of parallelism: events may be processed in many different cores at the same time.

For a comprehensive review about GPU proton dose calculations see: *Jia et al. Proton therapy dose calculations on GPU: advances and challenges. Transl. Canc Res. (2012). 1, 207-16.*

New Technological Developments for Fast Calculations: the GPU MC - 2

Limits such as the size of global and shared memory, maximum number of threads per block, and number of stream multiprocessors are GPU dependent. In the case of MC simulations, there exist some limitations to the effective number of parallel threads in a GPU. The large number of cores (typically thousands) cannot, in practice, be totally exploited at all times.

However, the achievable gain factor remains in any case significant.

Programming mostly in C/C++, using the CUDA® (Compute Unified Device Architecture) platform or the OpenCL (Open Computing Language) software libraries

Example of a GPU MC for medical applications: FRED (Fast paRticle thErapy Dose evaluator)

SAPIENZA UNIVERSITÀ DI ROMA

Maastro

THE HENRYK NIEWODNICZAŃSKI INSTITUTE OF NUCLEAR PHYSICS POLISH ACADEMY OF SCIENCES

PAUL SCHERRER INSTITUT PSI

Implementation and functionality

Commissioning and validation

iba MEVION medical systems VARIAN medical systems PAUL SCHERRER INSTITUT PSI

Fred protons

Applications

Quality assurance
Secondary dose calculation engine

Treatment planning studies
Multi-parameter studies on patient data

Treatment planning
Computation of dose, LET, vRBE

PET imaging
Simulations of proton beam induced beta+ activity

Proton CT imaging

Ongoing developments

Treatment plan optimization

4D applications

FRED Electromagnetic

FRED Carbon

antoni.rucinski@ifj.edu.pl

A. Schiavi et al. 2017 Phyd. Med. Biol. 62 7482

www.fred-mc.org Fred

FRED for research and QA in Proton Therapy

Fast pa**R**ticle th**E**rapy **D**ose Evaluator

Physics implementation

- Models contributing to dose in proton therapy
  - Proton tracking
  - Local deposition (heavy ions, delta rays)
- II class Monte Carlo algorithm
  - Condensed history
    - tabulated total stopping power (PSTAR-NIST)
    - energy straggling (Gaussian+Landau-Vavilov)
    - MCS models (Gauss+Rutherford)
  - Step-by-step implementation of nuclear interactions (elastic and inelastic, fragmentation)

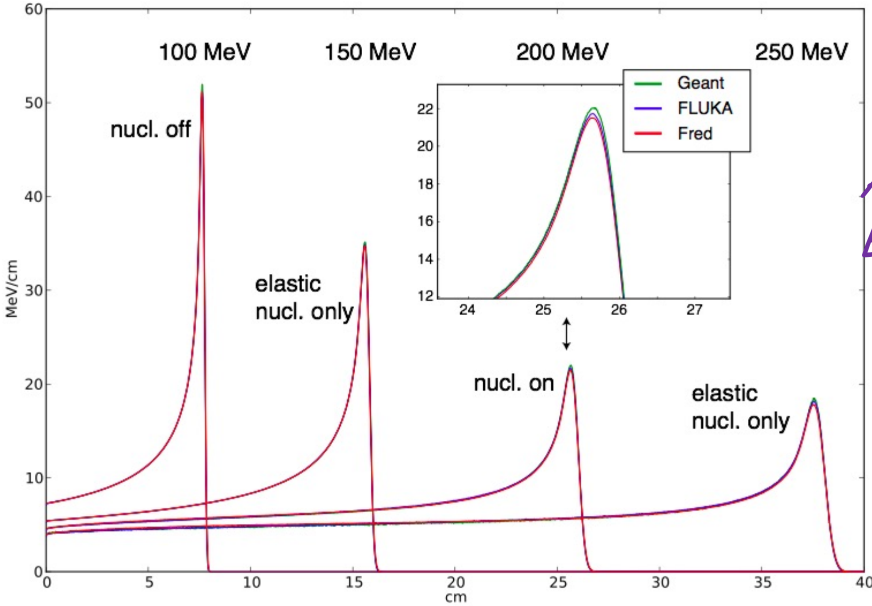
Validated against FLUKA

Functionality

- Speed: 1000x faster than general purpose MC
- CT import: HU to density conversion (Schneider-Parodi)
- Flexible voxelized geometry (CT+multiple user defined structures)
- Calculations of dose, LET, and vRBE (McNamara, Wedenberg, Carabe, Wilkens, Chen, etc.)
- Executable on multi-CPU/GPU systems and clusters
- Dose optimization
- C++ plugins

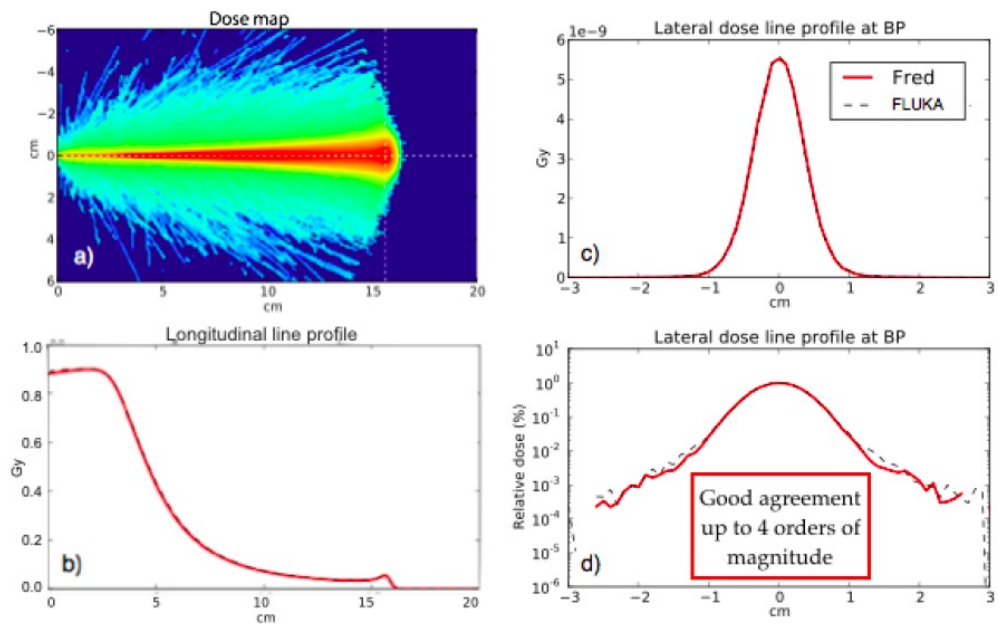
Accuracy, time performance, flexibility

FRED performances



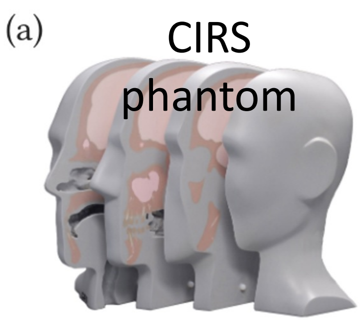
A. Schiavi et al. 2017 Phyd. Med. Biol. 62 , 7482

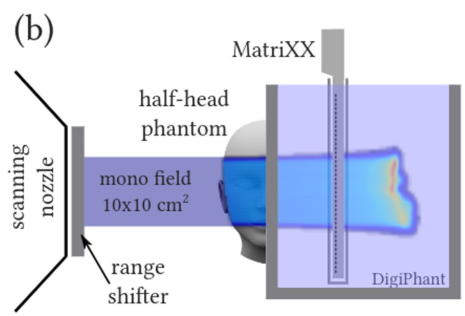
MC	Hardware	Primary/s	μs/primary
FLUKA	single CPU core	0.75k	1340
FRED	single CPU core	15k	68
FRED	single GPU cards	800k	1.35
FRED	4 GPU cards	20000k	0.05

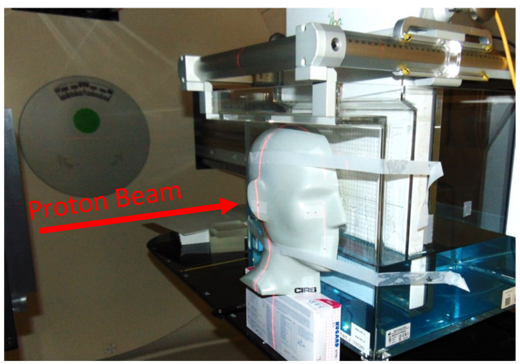


FRED experimental validation

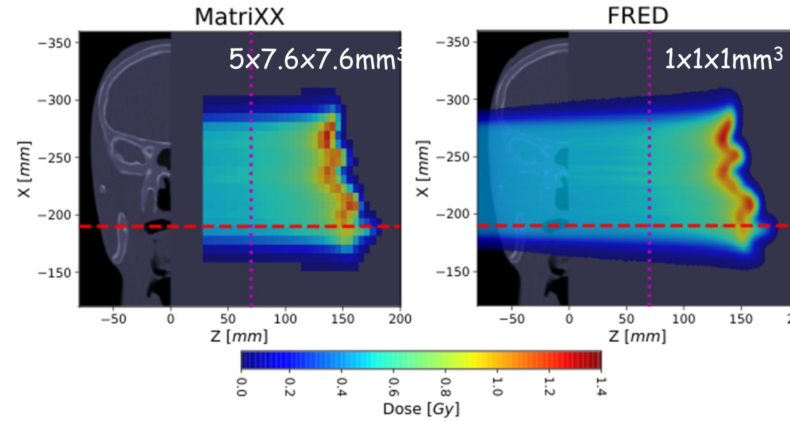
Collaboration with the proton therapy center of Kracow, Maastro and PSI

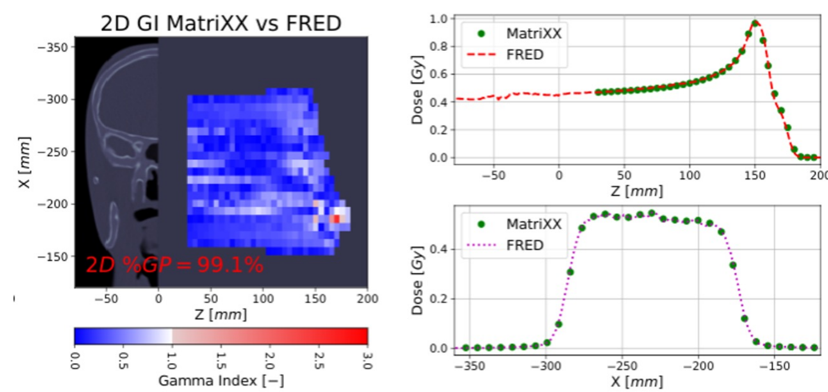






Mono layers: 100/150/200 MeV





3D GI pass rate (2%/2 mm/2%) >99%

J. Gajewski et al., Front. Phys. (2020)

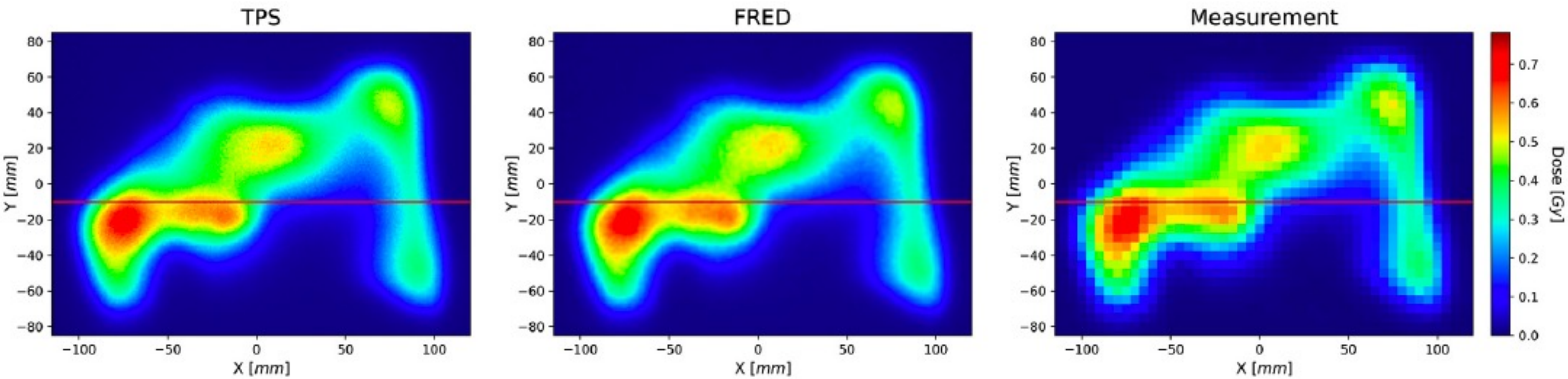
FRED clinical use

Collaboration with the proton therapy center of Kracow, Maastro and PSI

Implementation of a Compact Spot-Scanning Proton Therapy System in a GPU Monte Carlo Code to Support Clinical Routine

Front. Phys. 8 (2020) 578605

*Jan Gajewski[1], Angelo Schiavi[2,3], Nils Krah[4,5], Gloria Vilches-Freixas[6], Antoni Rucinski[1], Vincenzo Patera[2,3] and Ilaria Rinaldi[6]**



APPENDIX 1: HOW TO INTERFACE RADIOBIOLOGICAL DATABASES

Biologically Oriented Scoring in FLUKA*

For each **energy deposition i,** FLUKA interpolates from the external database provided by the user the **$\alpha_{D,i}$ and $\beta_{D,i}$** parameters for the specific ion with a certain charge at a certain energy.
Then **FLUKA sums up** properly **the mixed radiation effect** applying the Kellerer and Rossi theory of dual radiation action:

$$\sum \alpha_{D,i} D_i \qquad \sum \sqrt{\beta_{D,i}} D_i$$

Then the **average biological parameters** can be calculated at the end of the FLUKA run:

$$\overline{\alpha} = \frac{\sum \alpha_{D,i} D_i}{\overline{D}} \quad \text{and} \quad \overline{\beta} = \left(\frac{\sum \sqrt{\beta_{D,i}} D_i}{\overline{D}} \right)^2 \quad \text{with} \quad \overline{D} = \sum D_i$$

For example the **cell survival** can be calculated:

See talk by A. Mairani ID 64

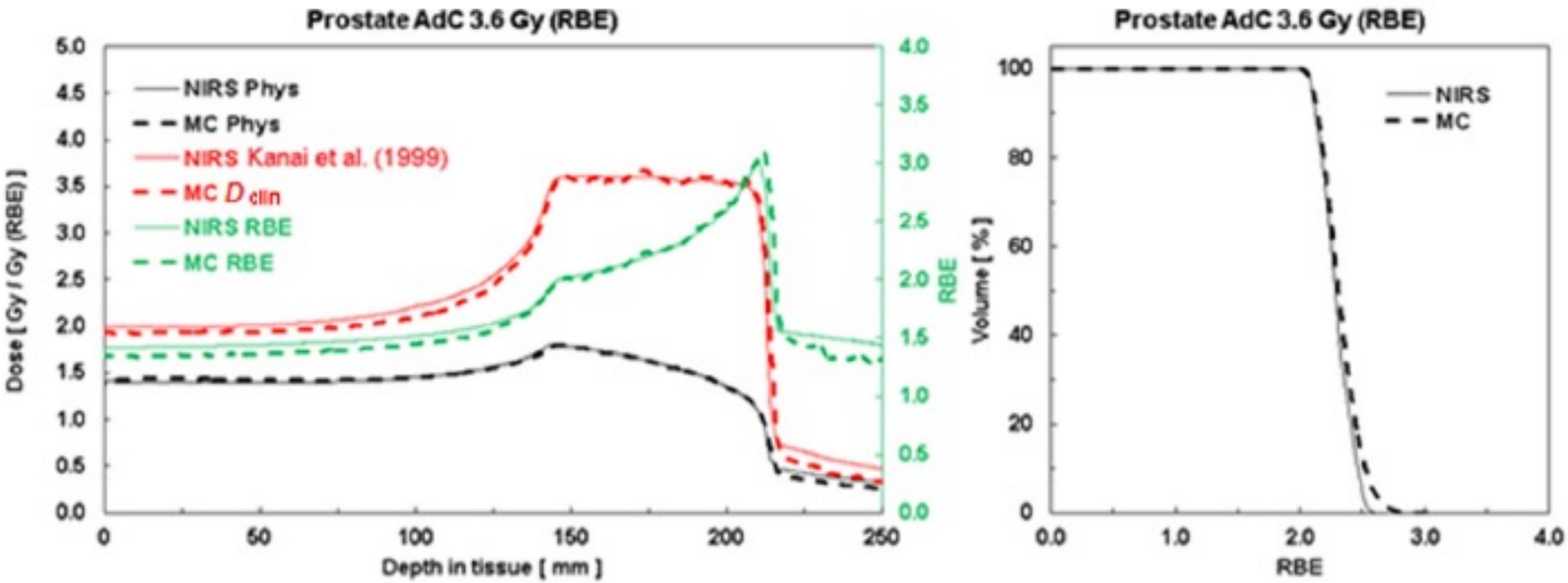
$$S = \exp(-\overline{\alpha}\,\overline{D} - \overline{\beta}\,\overline{D}^2)$$

Phys. Med. Biol. 62 (2017) 3814

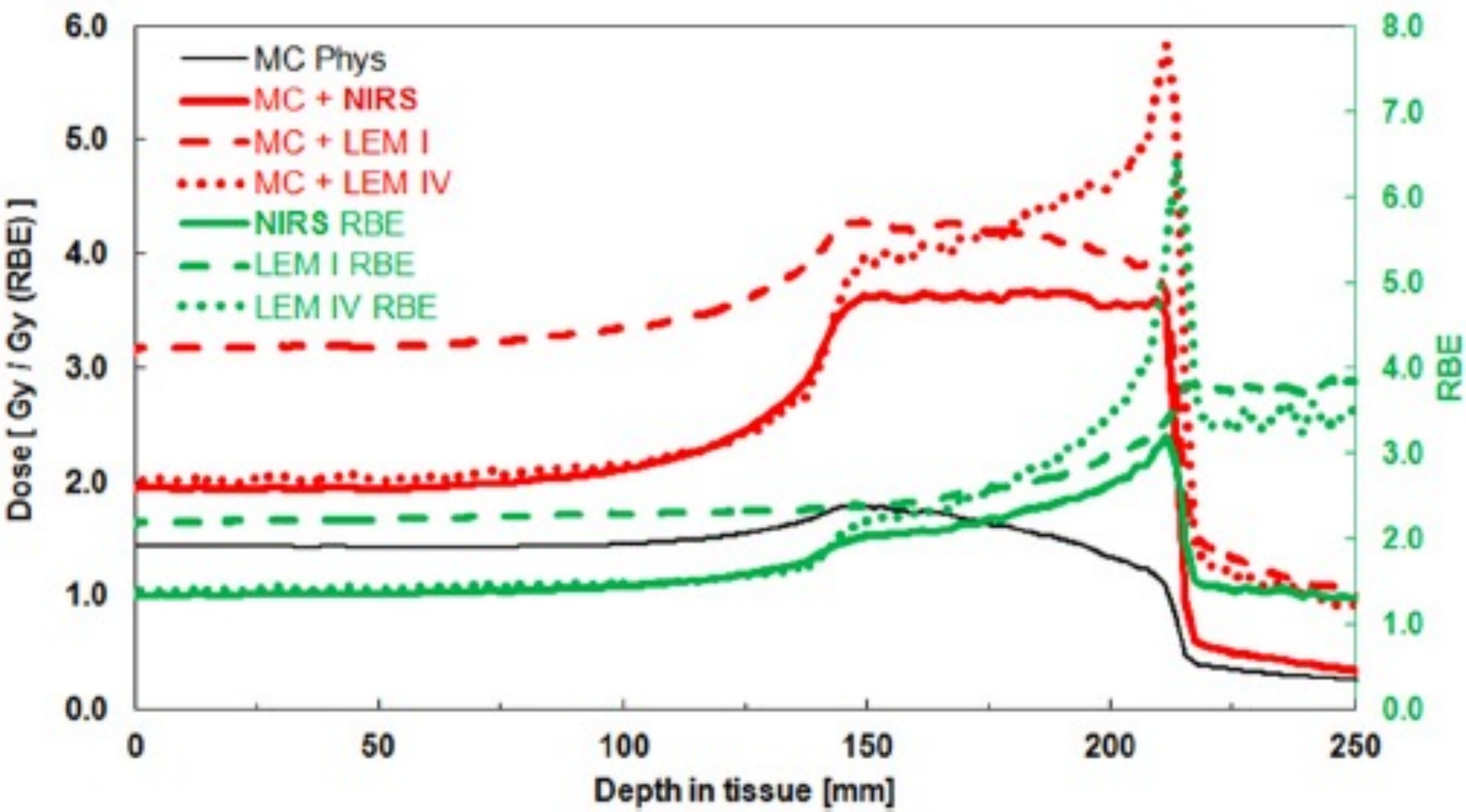
The FLUKA Monte Carlo code coupled with the NIRS approach for clinical dose calculations in carbon ion therapy

CNAO

G Magro[1], T J Dahle[2], S Molinelli[1], M Ciocca[1], P Fossati[1,3], A Ferrari[4], T Inaniwa[5], N Matsufuji[5], K S Ytre-Hauge[2] and A Mairani[1,6]



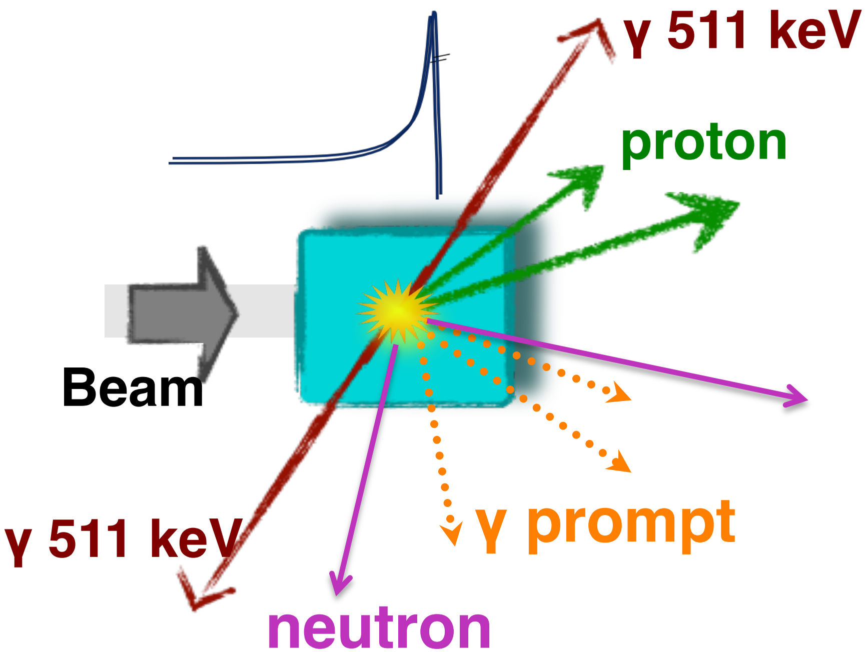
MC tools which allow flexible determination of the biological effect based on various radiobiological models to guarantee a fair comparison between clinical RBE-weighted dose data based on different calculation systems.



Comparison of **effective dose profiles** acquired at the isocenter in the target volume for a prostate AdC (3.6 Gy (RBE)), as computed by the NIRS approach (solid line), the LEM I (dashed line) and LEM IV (dotted line) model coupled with the FLUKA MC code. The corresponding **physical dose profile** is also shown, together with **RBE depth profiles**

APPENDIX 2:
FLUKA APPLICATION TO RANGE MONITORING IN HANDRONTHERAPY

In vivo verification



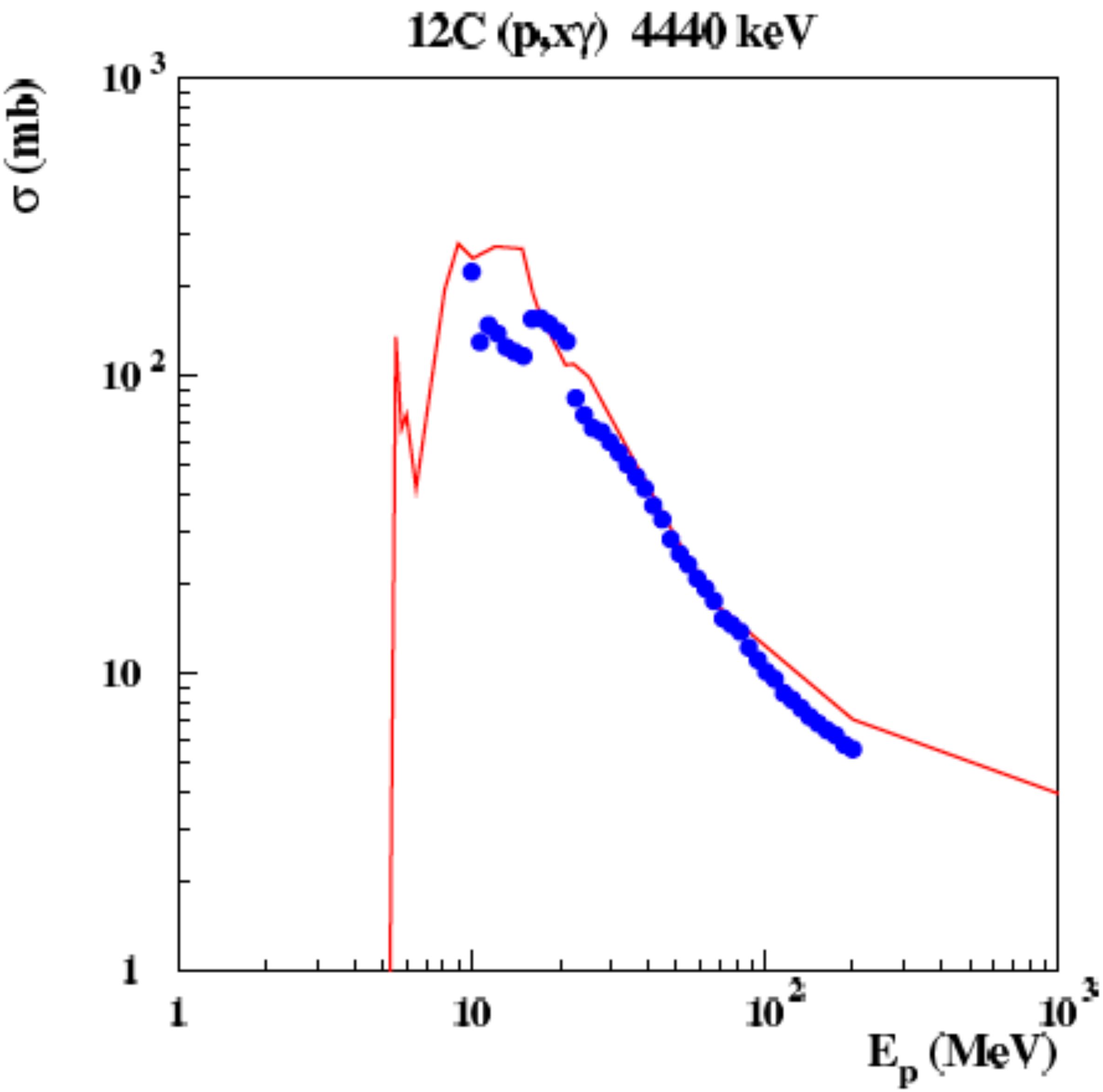
see talks by
E. Fiorina (ID 143)
and
S. Muraro (ID 67)

Secondary particle production during treatment can be used to perform range monitoring *(and maybe dose monitoring)*

Correlation of measurements of secondary particles with the spatial profile of dose deposition is performed/understood by means of comparison with MC predictions

FLUKA can be successfully used for this purpose

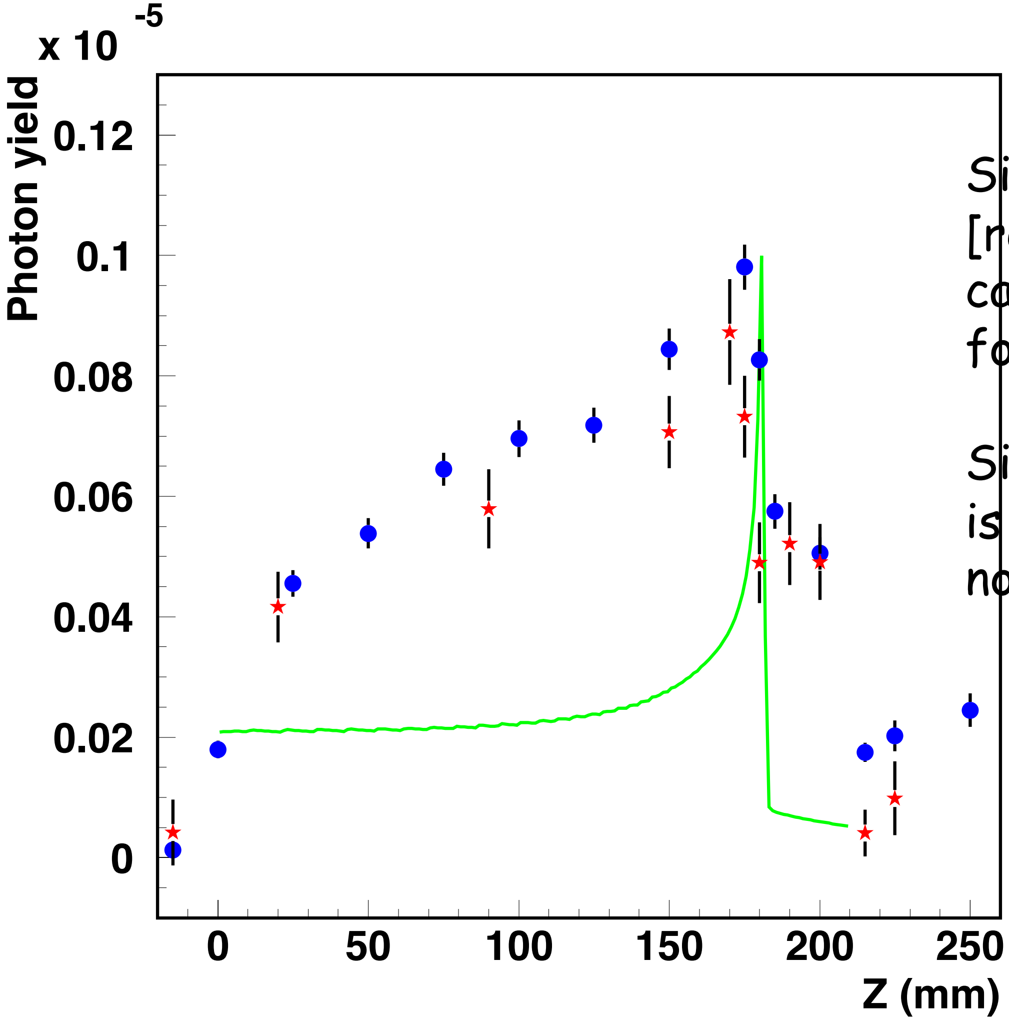
De-excitation (prompt) γ production



Excitation function for the emission of the discrete 4.440 MeV *γ* line from proton-induced reactions on carbon

de-excitation of
the 1st excited level in ^{12}C,
the 2nd excited level in ^{11}B,
the 2nd excited level in ^{11}C.

In vivo verification: prompt γ's



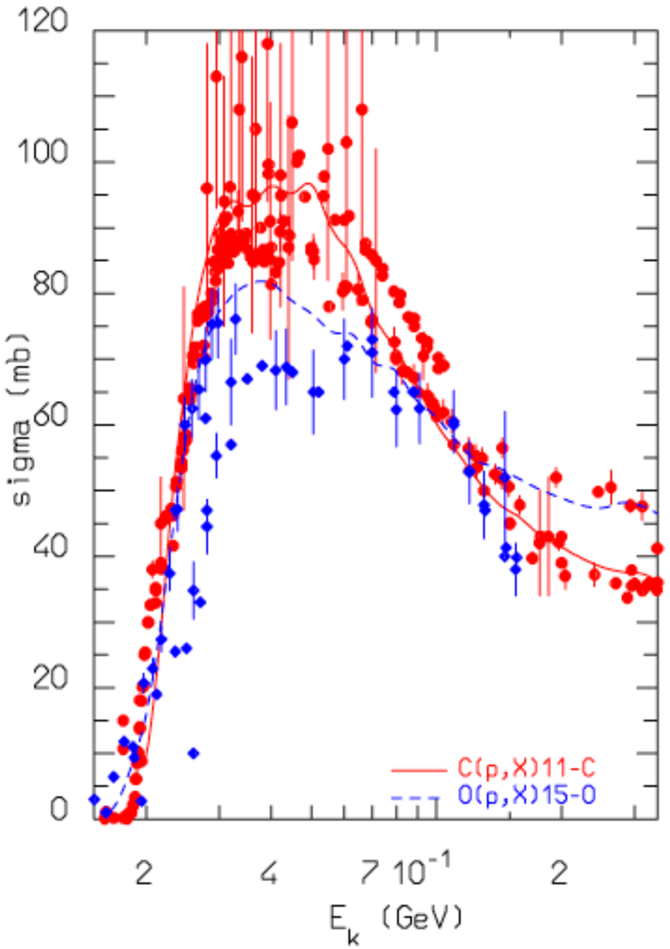
Simulated (blue circles) and measured [red asterisks] data are shown for carbon ion beam at 310 MeV/n for setup SIII (right, on water).

Simulated depth-dose distribution is also shown with arbitrary normalization.

E. Testa Personal Communication, Data Shared on the FP7-ENVISION project Internal Website. (2012).

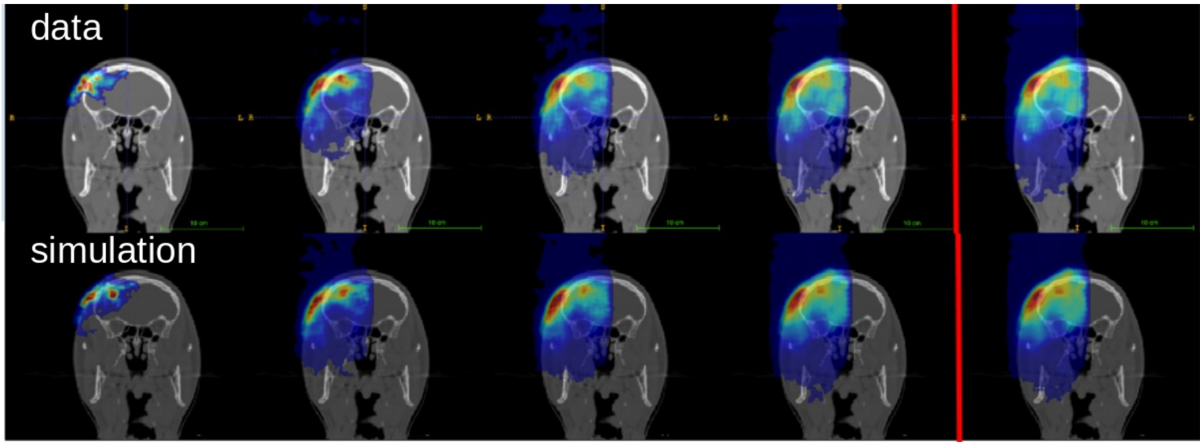
ENVISION

About PET in-beam prediction capability



FLUKA predictions for the reactions $^{nat,12}C(p,x)^{11}C$ and $^{nat,16}O(p,x)^{15}O$ cross sections as a function of projectile energy, compared against data retrieved from the eXFOr library

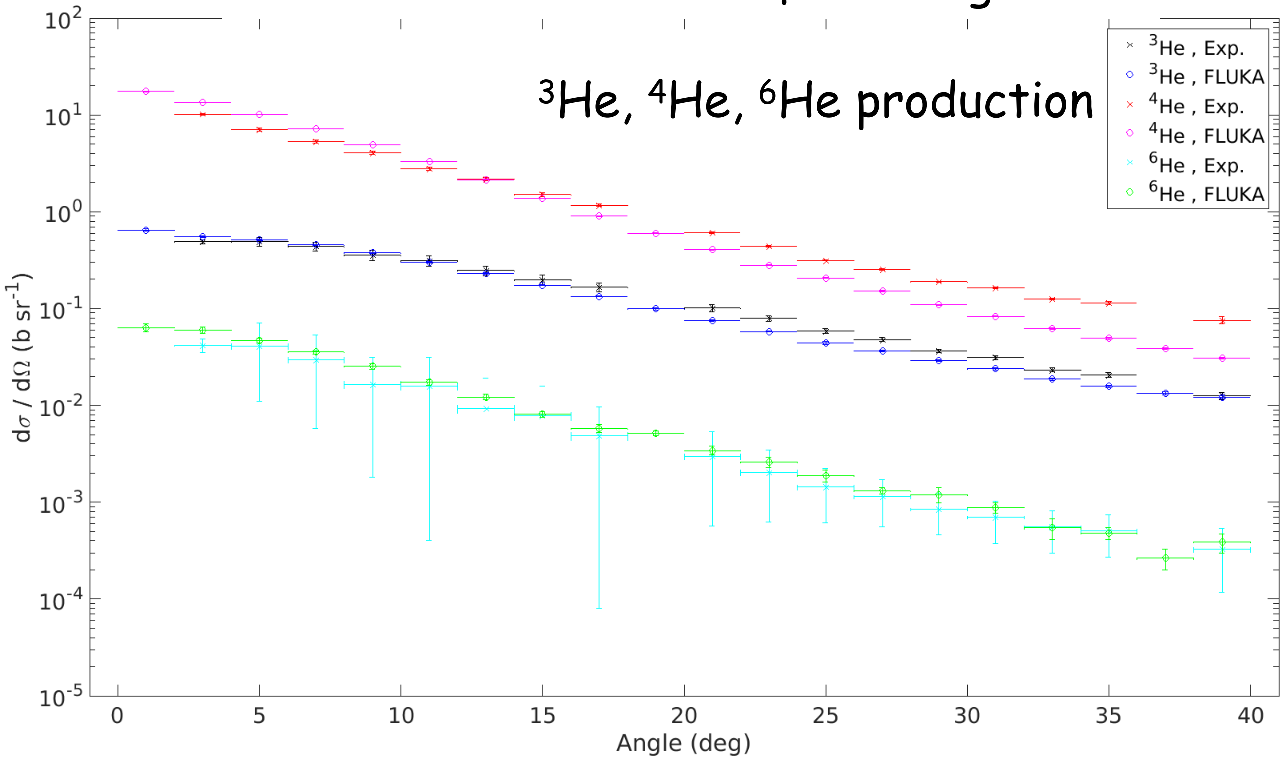
A clinical case



Charged particle production

50 MeV/u 12C on a 250 µm C target

G. Aricò (CERN/OMA)



Fluka vs Exp

Compare:

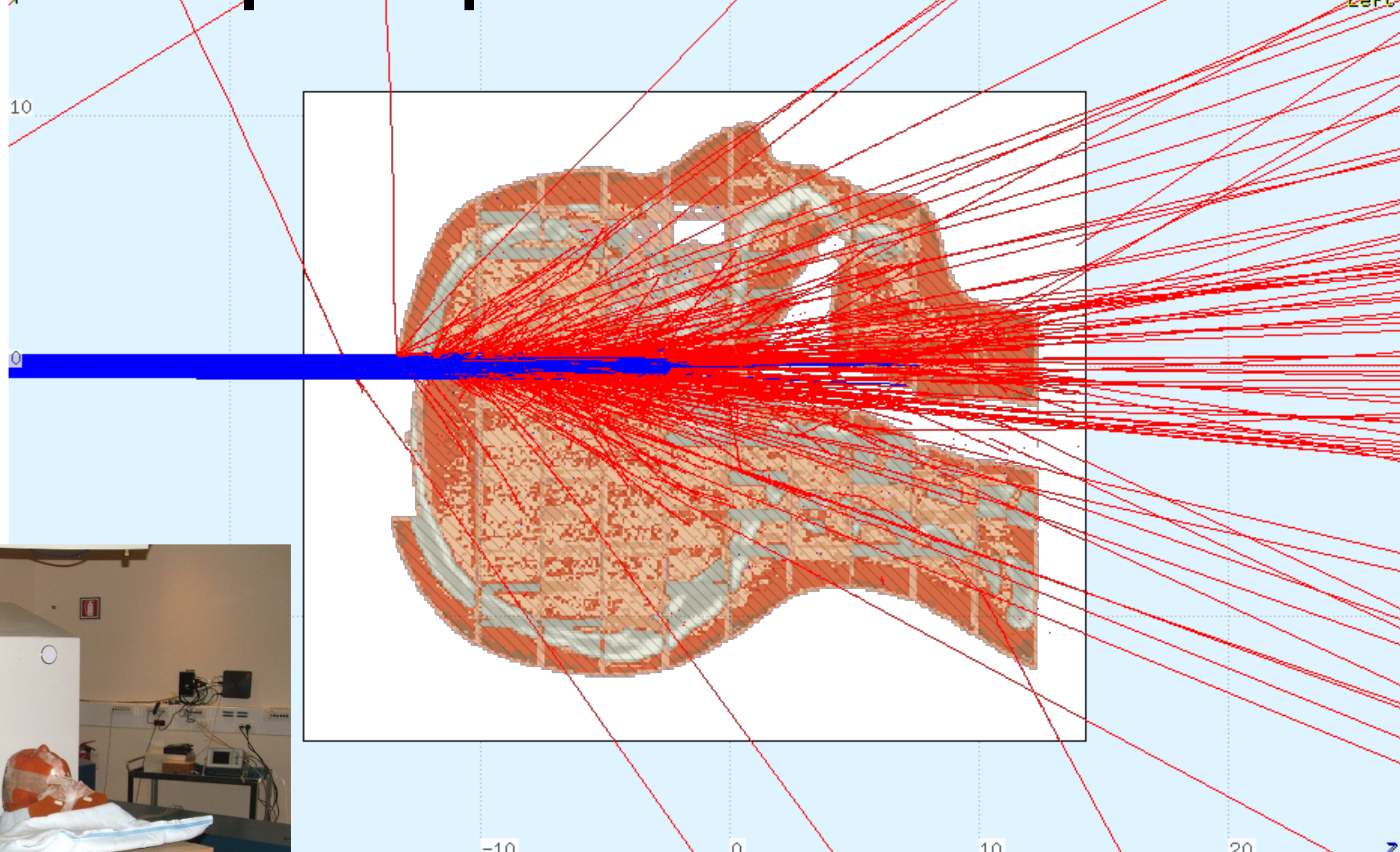
Blue - Black

Magenta - Red

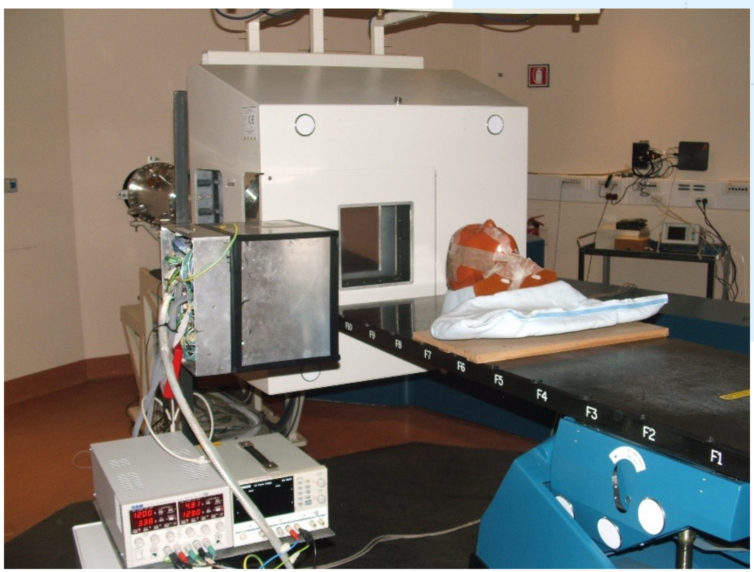
Green - Cyan

Exp. C. Divay et al, Phys. Rev. C95 (2017)

Simulation of CNAO 12C beam at 220 MeV/u on Antropomorphic Phantom



InSide



see talk by S. Muraro ID 67