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Introduction to Monte Carlo Radiation Transport Codes

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Outline

- Introduction
- Interactions of Fast Particles with Matter and Materials under Irradiation
- Monte-Carlo (MC) Method in Particle Transport in Matter
- Total and Differential Cross-sections and Event Generators
- Quasi-Continuous Effects
- MC Simulation Scheme
- Radiation Damage, DPA etc.
- Five General-Purpose MC Codes: Features and Examples
- Benchmarking and Code Inter-comparison
- How to Get the Best out of the MC Codes

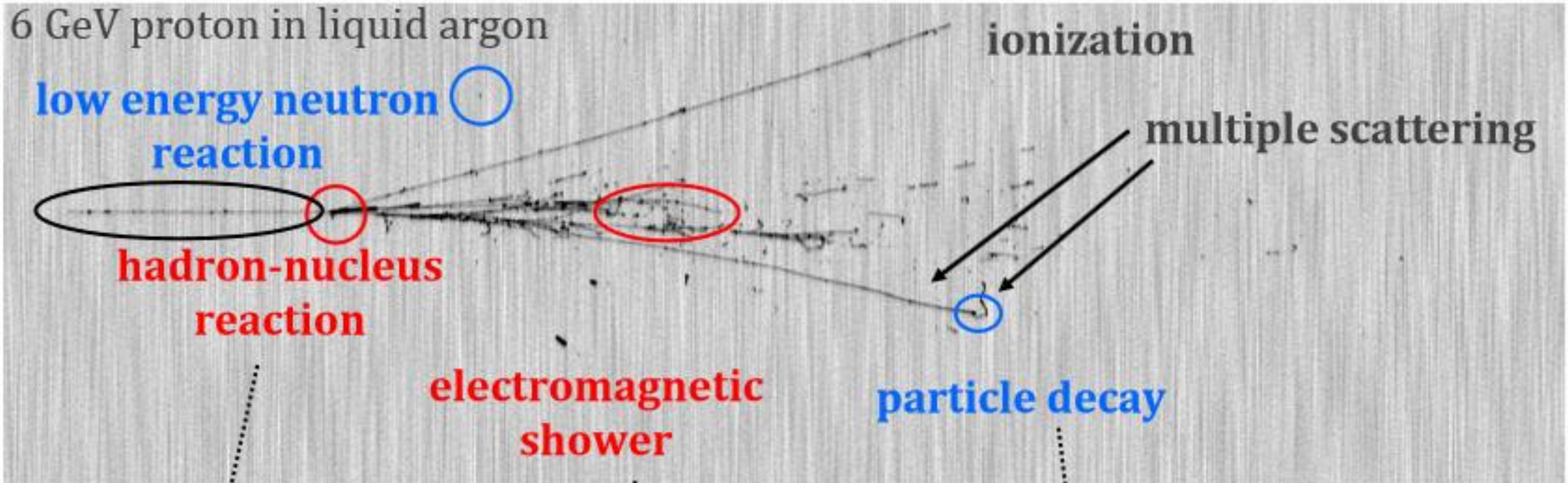
Introduction

The consequences of controlled and uncontrolled impacts of high-intensity or/and high-power or/and high-energy beams on components of accelerators, beamlines, target stations, beam collimators, absorbers, detectors, shielding, and environment can range from minor to catastrophic.

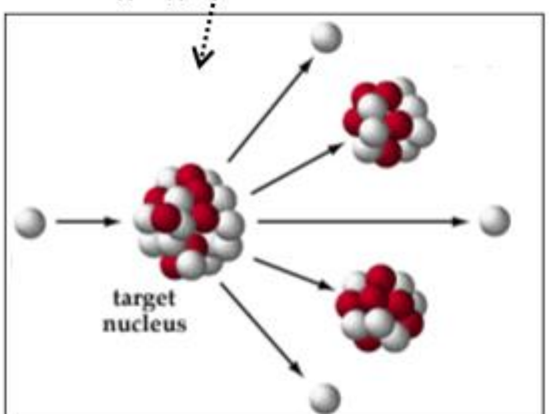
Strong, weak, electromagnetic and even gravitational forces (neutron oscillation and neutron TOF experiments) govern high-energy beam interactions with complex components in presence of electromagnetic fields ➔ simulations are only possible with a few well-established Monte-Carlo codes (no analytic or simplified approaches are used these days).

Predictive power and reliability of particle transport simulation tools and physics models should be well-understood and justified to allow for facility upgrades and viable design of future setups with a minimal risk and a reasonable safety margin.

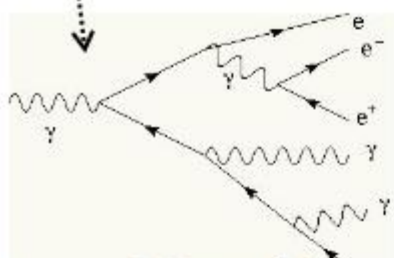
Microscopic View



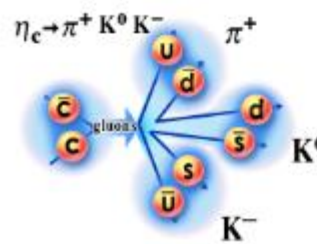
$$\lambda\rho = \frac{A}{\sigma_R N_A} \qquad \sigma_R \simeq \pi r_0^2 A^{2/3}$$



interplay of many physical processes described by different theories/models



$$X_0\rho \simeq \frac{716.4\ g\ cm^{-2}\ A}{Z(Z+1)\log(287/\sqrt{Z})}$$



Materials Under Intense Irradiation

Depending on material, level of energy deposition density and its time structure, one can face a variety of effects in materials under impact of directly particle beams or radiation induced by them.

Component damage (lifetime):

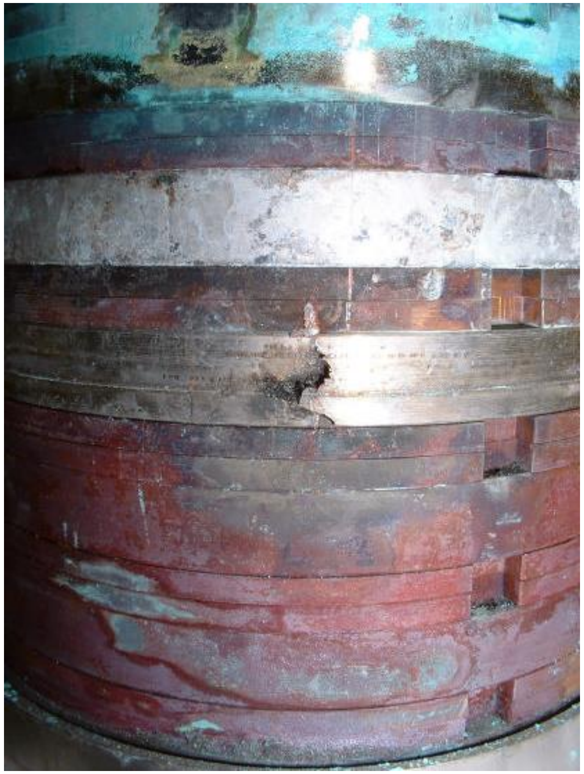
- Thermal shocks and quasi-instantaneous damage
- Insulation property deterioration due to dose buildup
- Radiation damage to inorganic materials due to atomic displacements and helium production

Operational (performance):

- Superconducting magnet quench
- Single-event upset and other soft errors in electronics
- Detector performance deterioration
- Radioactivation, prompt dose and impact on environment

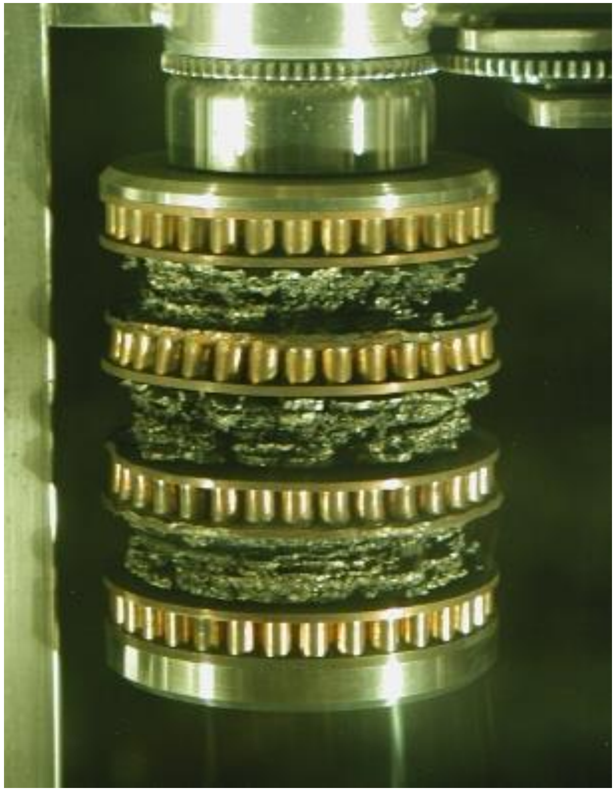
Thermal Shock

Short pulses with energy deposition density EDD in the range from 200 J/g (W), 600 J/g (Cu), ~1 kJ/g (Ni, Inconel) to ~15 kJ/g: thermal shocks resulting in fast ablation and slower structural changes.



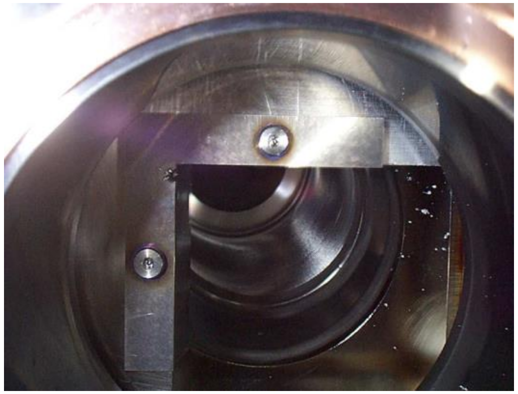
FNAL pbar production target under 120-GeV p-beam (3e12 ppp, σ ~ 0.2 mm)

MARS simulations explained target damage, reduction of pbar yield and justified better target materials

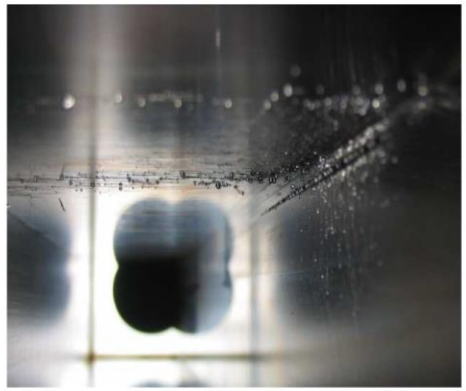


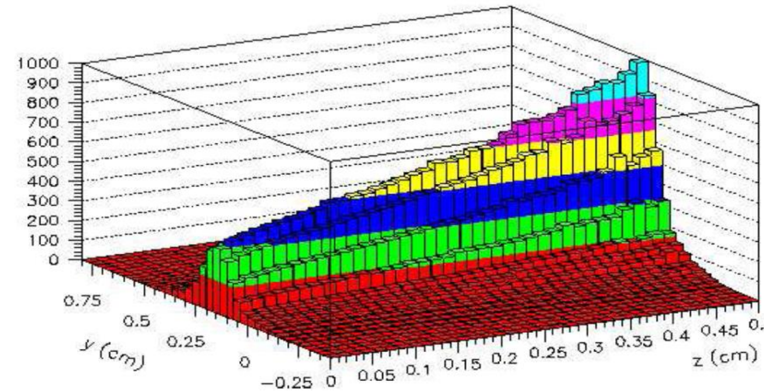
Tevatron Tungsten Collimator Ablation

Hole in 5-mm W



25-cm groove in SS





Detailed modeling of dynamics of beam loss (STRUCT), energy deposition (MARS15) as high as 1 kJ/g, and time evolution over 1.6 ms of the tungsten collimator ablation, fully explained what happened

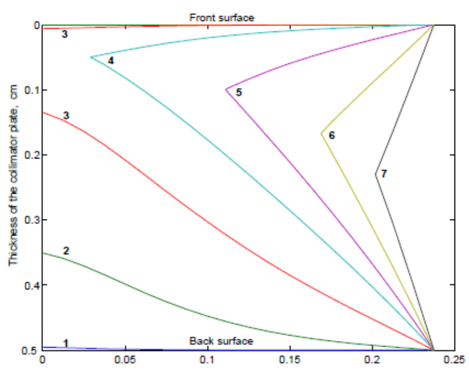
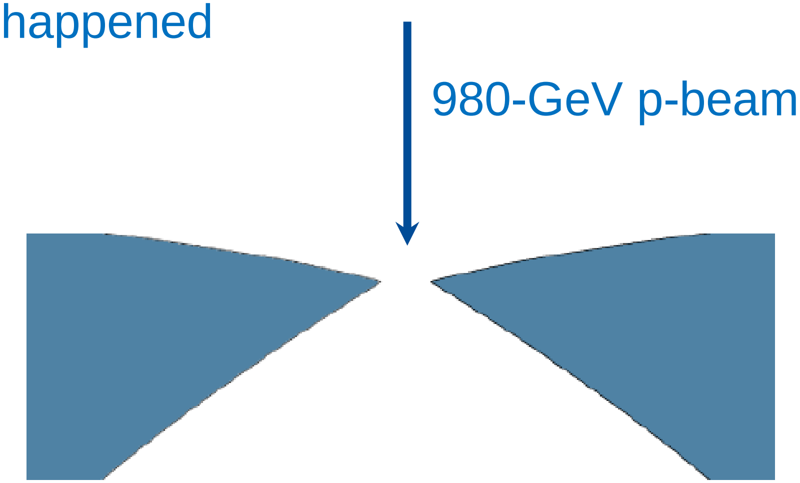


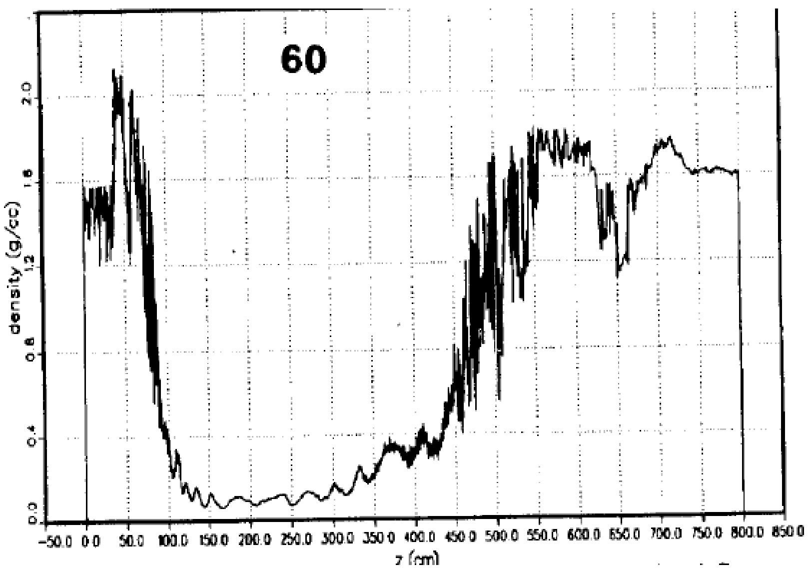
Figure 7: Evolution of the front and back surfaces of the collimator plate at $t = 0.4_{[1]} - 1.6_{[7]}\ ms$ with Δt=0.2 ms.



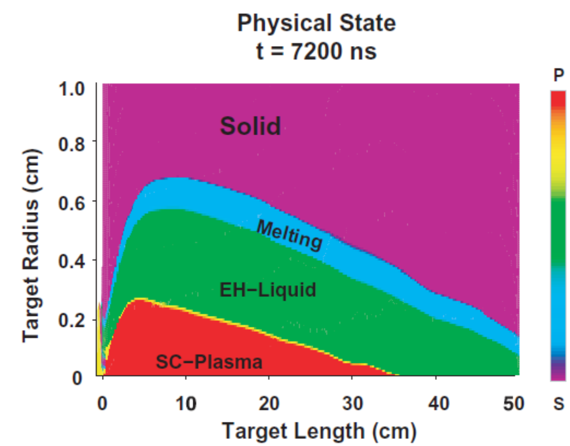
Hydrodynamic Tunneling in Solid Materials

Pulses with EDD >15 kJ/g: hydrodynamic regime.

First done for the 300-μs, 400-MJ, 20-TeV proton beams for the SSC graphite beam dump, steel collimators and tunnel-surrounding Austin Chalk by SSC-LANL Collaboration (D. Wilson, …, N. Mokhov, PAC93, p. 3090). Combining MARS ED calculations at each time step for a fresh material state and MESA/SPHINX hydrodynamics codes.



The hole was drilled at the 7 cm/μs penetration rate. Shown is axial density of graphite beam dump in 60 μs after the spill start



Later, studies by N. Tahir et al with FLUKA+BIG2 codes for SPS & LHC

We also used MARS+FRONTIER

Monte-Carlo Method in Particle Transport in Matter

Nowadays, the **Monte-Carlo method (MCM)** is the principal, if not the only, method in particle transport applications. In its simplest and at the same time most dependable and common form – ***direct mathematical modeling*** – it involves numerical simulation of the interactions and propagation of particles in matter. In this approach, all the physics processes are modelled as these take place in the real world, in realistic geometry and fields of accelerators and experimental setups.

The use of various modifications of MCM, the so--called ***variance reduction techniques***, makes it possible to greatly simplify the solution of the problem in certain cases, with a very high accuracy reached in a limited phase space volume.

Five Codes Widely Used Around the Globe

The use of **general-purpose particle interaction and transport Monte Carlo codes** is the most accurate and efficient choice for assessing impact and consequences of particle-matter interactions at accelerators. Due to the vast spread of such codes to all areas of particle physics and the associated extensive benchmarking with experimental data, **the modeling has reached an unprecedented accuracy**.

Furthermore, most of these codes allow the user to simulate all aspects of a high energy particle cascade in one and the same run: from the first interaction of a primary beam (of up to TeV energies) over the transport and re-interactions (hadronic and electromagnetic) of the produced secondaries, to detailed nuclear fragmentation, the calculation of radioactive decays, secondary electromagnetic showers, muon and neutrino generation and their interaction with surroundings.

Principal features and examples are given in the rest of the talk for

FLUKA, GEANT4, MARS15, MCNP6 and PHITS

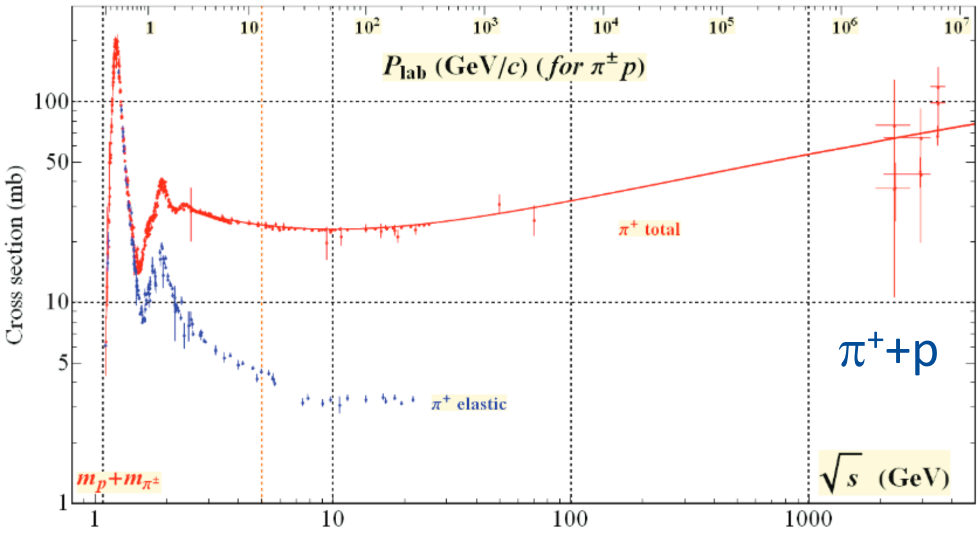
Fermilab

Nuclear Interaction Cross-Sections

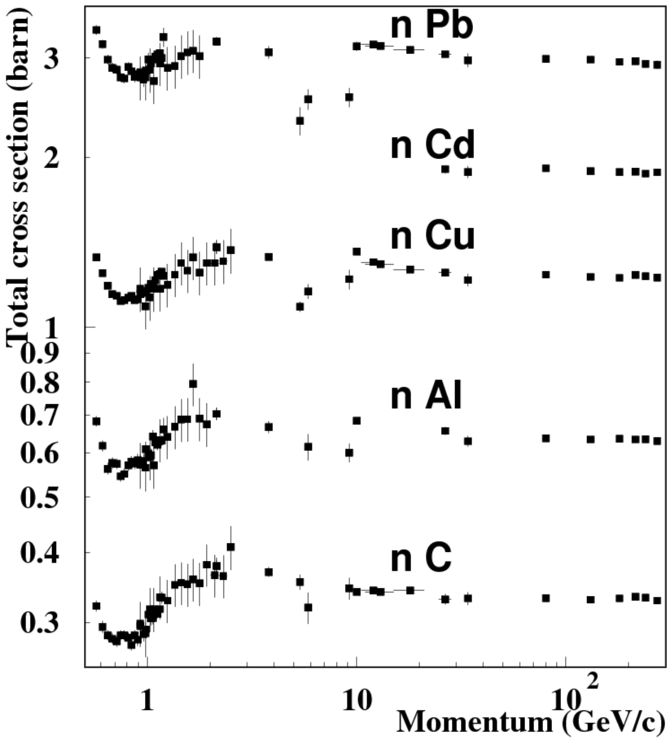
The **first most important quantity** to simulate particle transport by Monte-Carlo method

$$\Sigma(i, A, E) = \frac{\sigma(i, A, E) N_A 10^{-27} \rho}{A}, \text{ cm}^{-1}$$

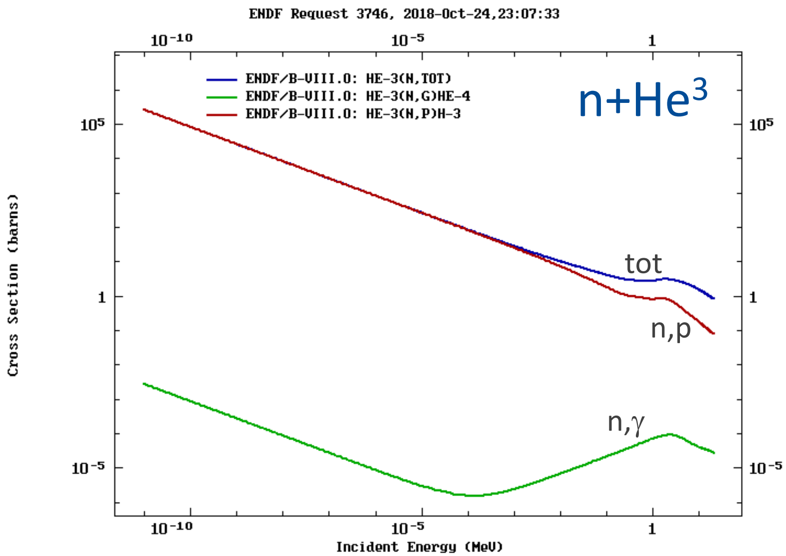
where σ is a microscopic x-section (mb) for a given interaction type of a particle of *i*-type with a chosen absorber nucleus with atomic mass A; N_A is Avogadro number (=6.022$\times 10^{23}$ mol^{-1}), ρ is density (g/cm^3)

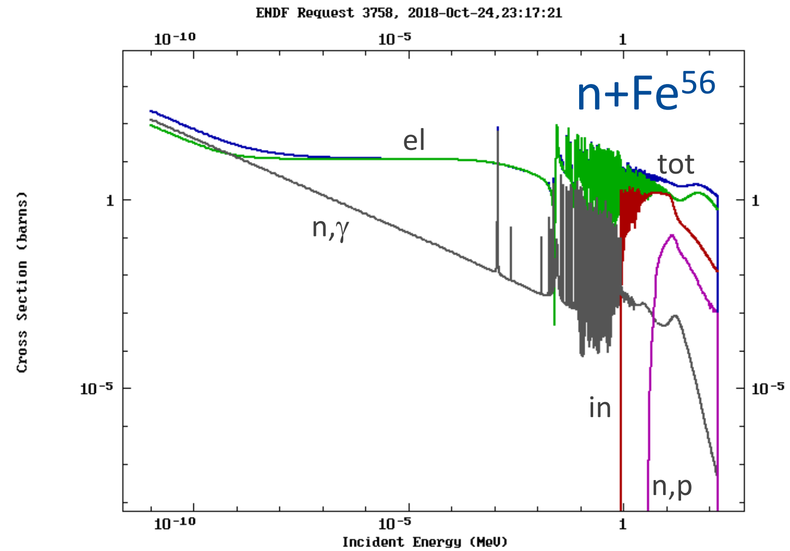


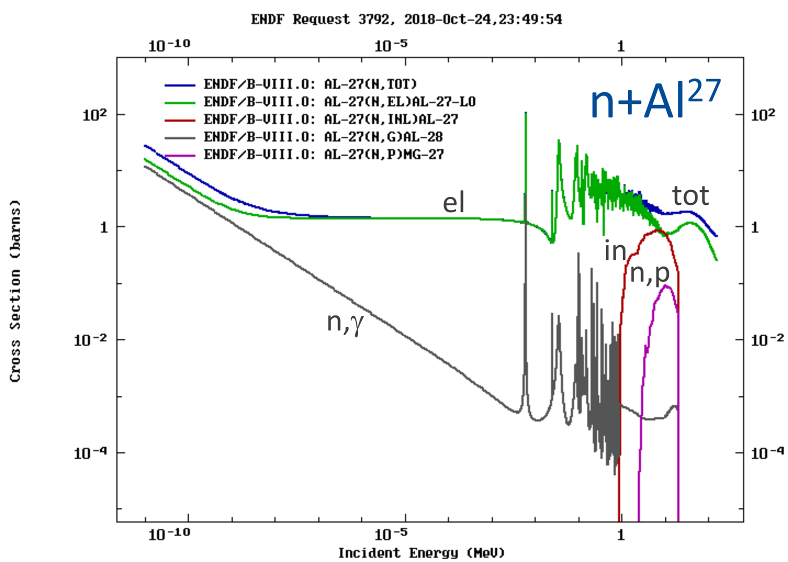
$$s = m_1^2 + m_2^2 + 2E_{1lab} m_2$$

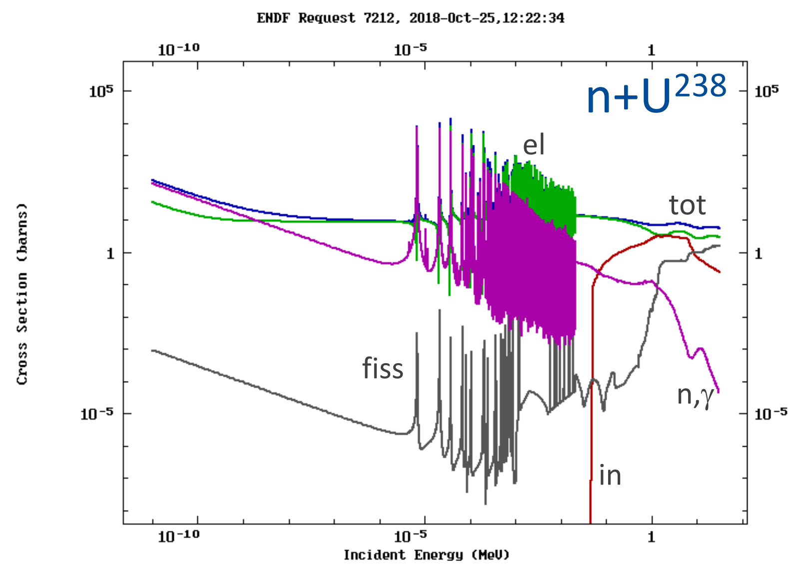


Low-Energy Neutron-Nucleus Cross-Sections









Double-Differential X-Section or Particle Production Models

The **second most important quantity** to simulate particle transport by Monte-Carlo method is a double-differential cross-section:

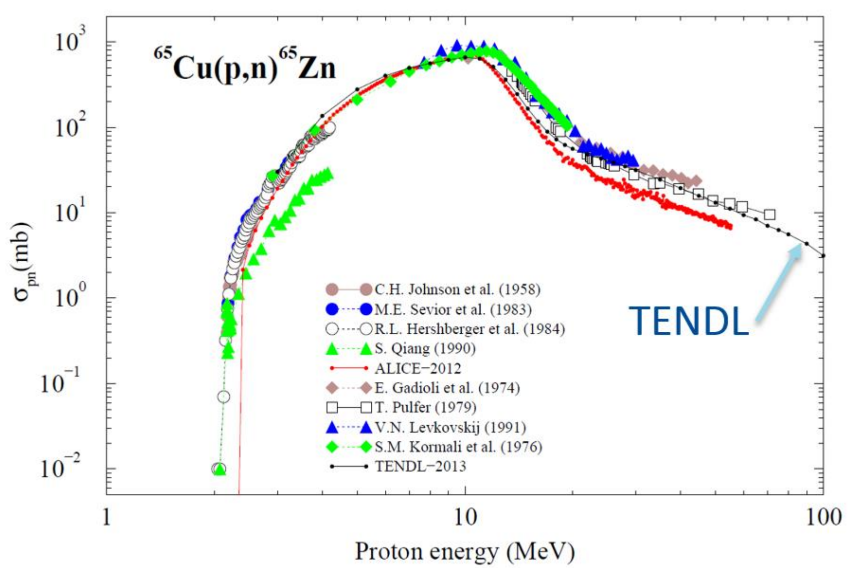
$$\Sigma(\vec{r}, \Omega' \rightarrow \Omega, E' \rightarrow E) = \frac{d^2\sigma(i,j,A,E',E,\Omega',\Omega)}{dE d\Omega} \times \frac{N_A 10^{-27} \rho}{A}$$

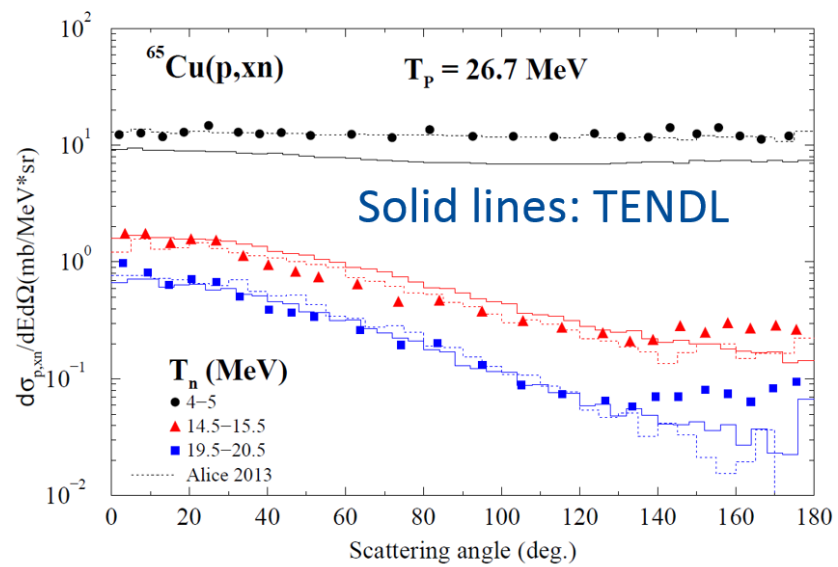
At intermediate and low energies, it can be taken from evaluated databases (e.g., ENDF for low-energy neutrons with their x-section resonant structure), or some theoretical forms.

At high-energies, a standard approach nowadays is to use ***event generators***, performing Monte-Carlo simulation through all the stages of particle interactions inside a nucleus like a quark-gluon cascade, hadron intranuclear cascade, preequilibrium stage, evaporation/fragmentation and gamma-deexcitation. This is realized, e.g., in DPMJET (Dual Parton Model), FRITIOF (string model), LAQGSM (quark-gluon string model), and QMD (Quantum Molecular Dynamics model).

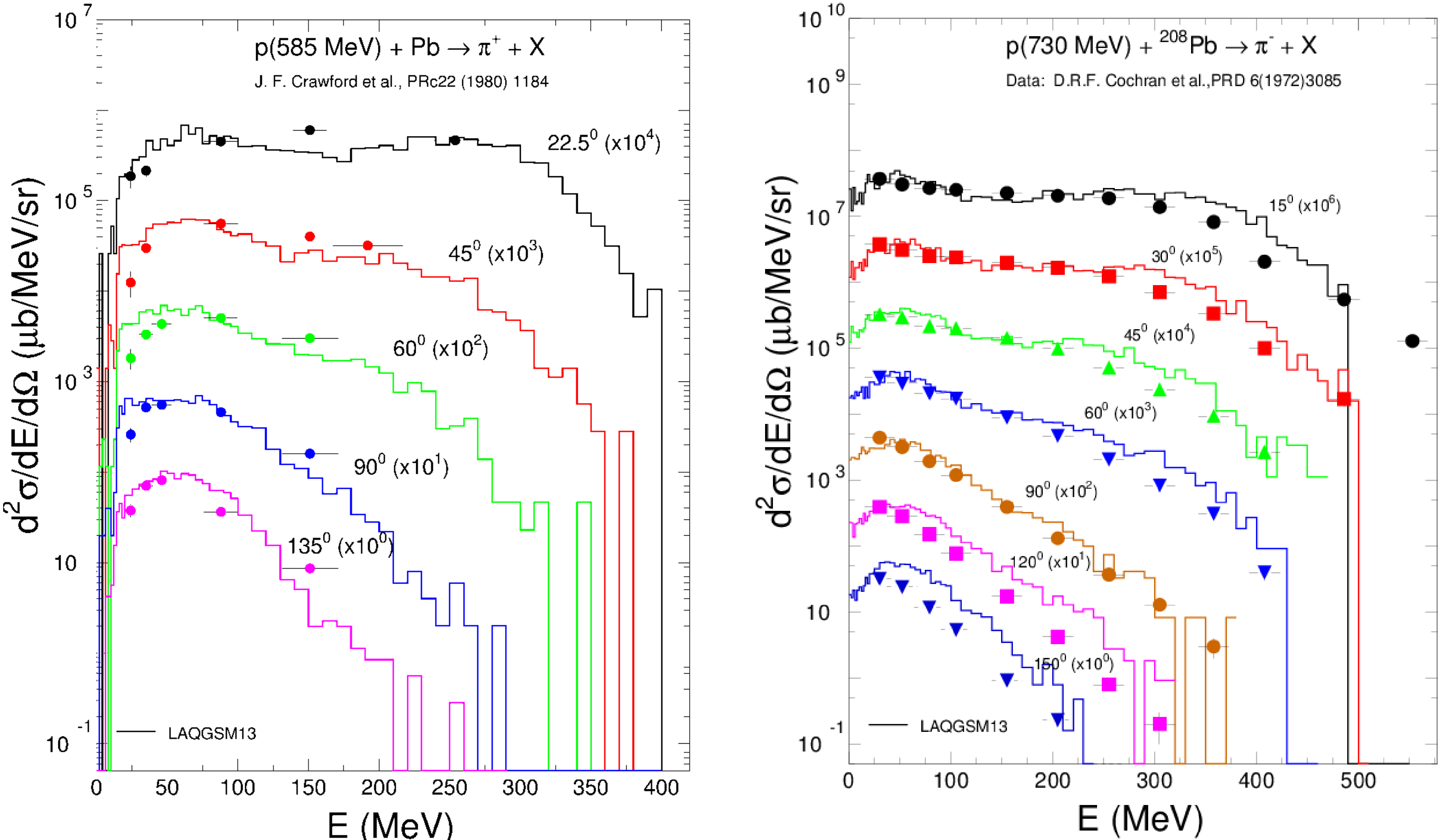
Example: MARS15 Nuclear Event Generator Set

- Projectile E_0 < 0.12 GeV down to 1 MeV (charged particles) and 14 MeV (neutrons): a combination of <u>extended</u> TENDL-2016 (inclusive, semi-inclusive or exclusive mode – user's choice) and LAQGSM
- 0.12 < E_0 < 0.5 GeV: a combination of CEM-2018 and LAQGSM-2018
- 0.5 < E_0 < 10 GeV: LAQGSM
- 10 GeV < E_0 < 100 TeV: LAQGSM or inclusive (user's choice)

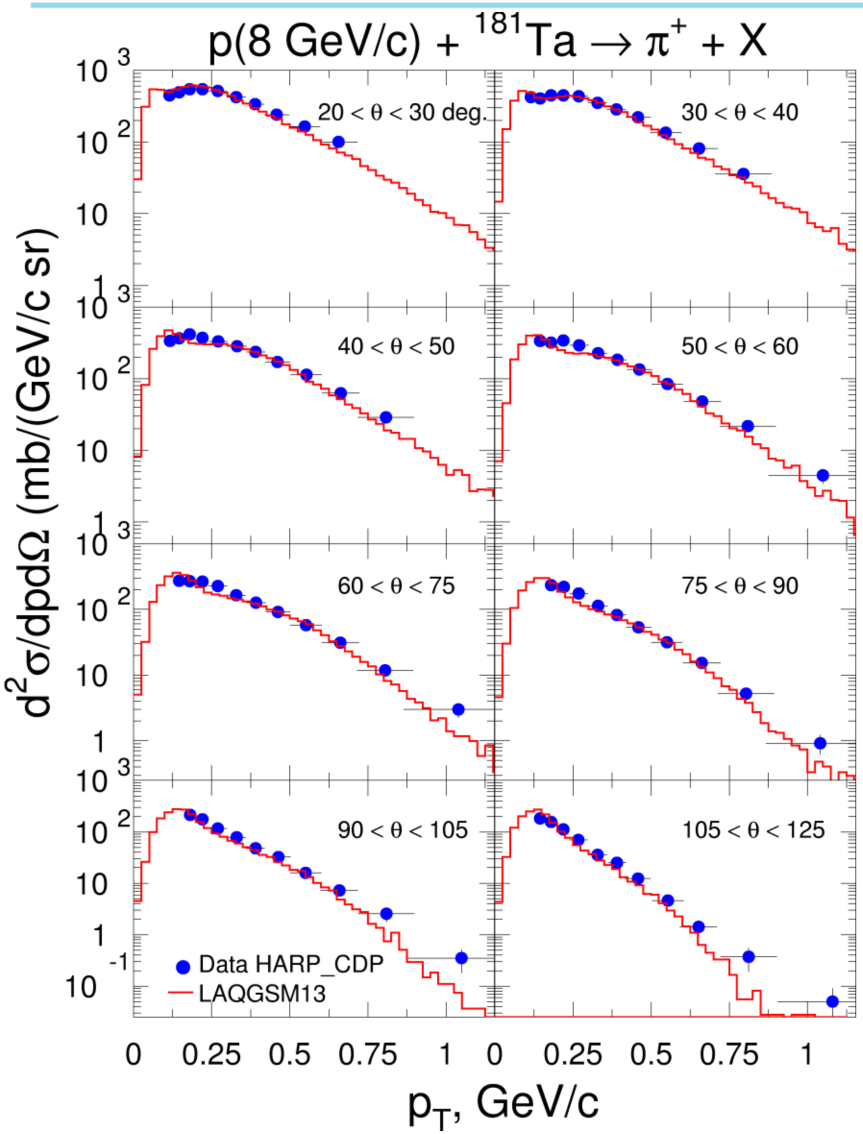


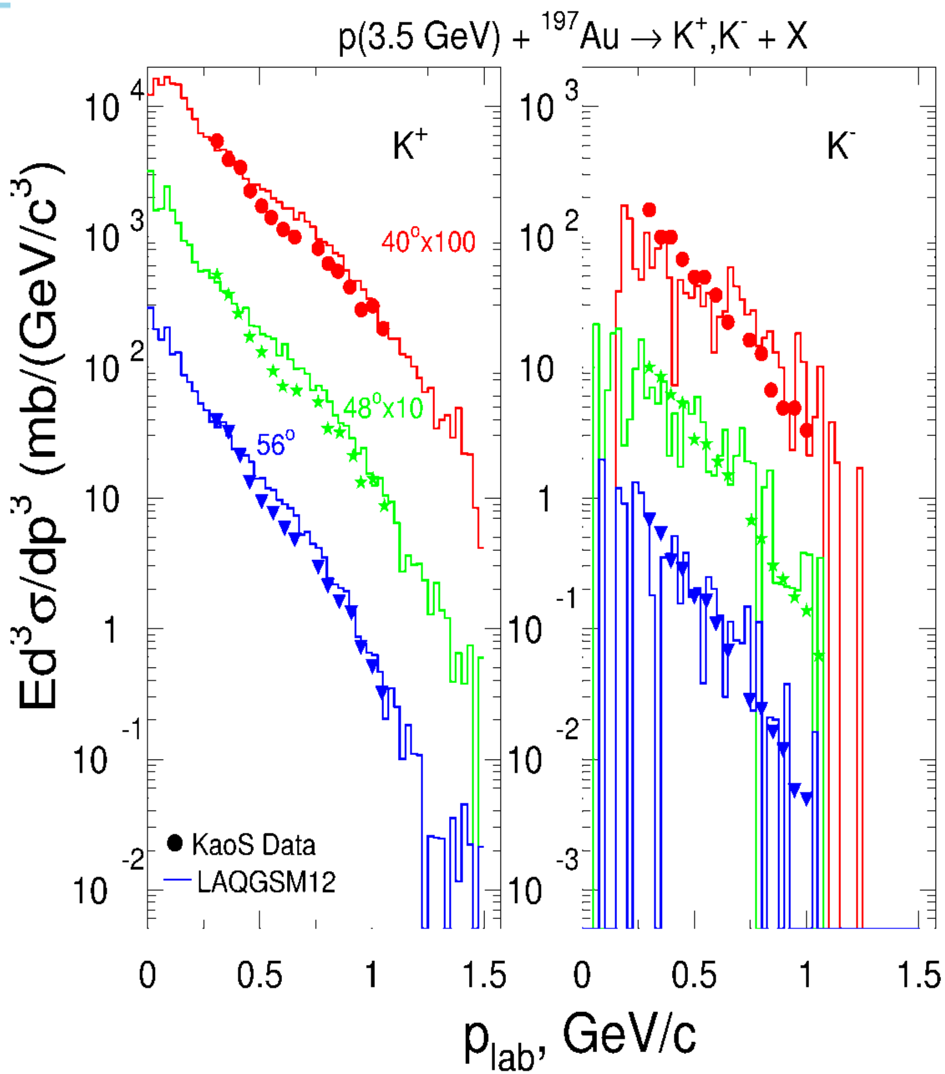


MARS-LAQGSM Performance at 585 and 730 MeV

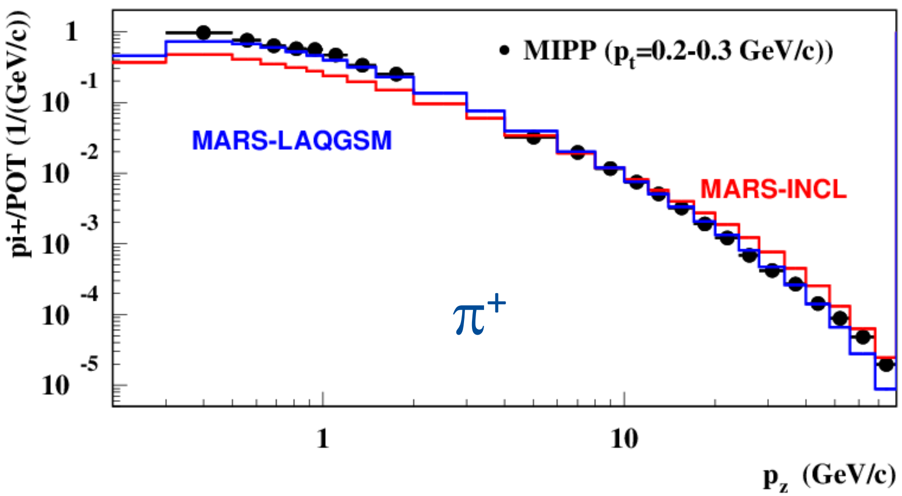


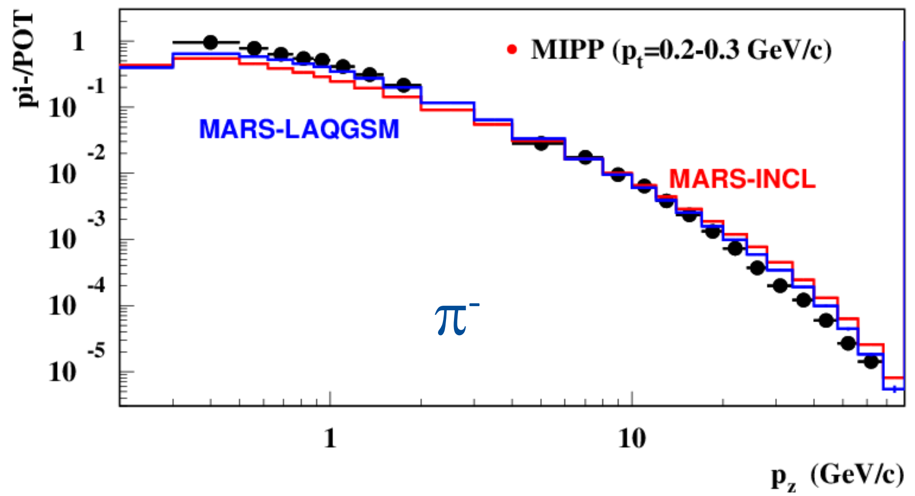
LAQGSM vs HARP-CDP at 8GeV/c and KaoS at 3.5GeV

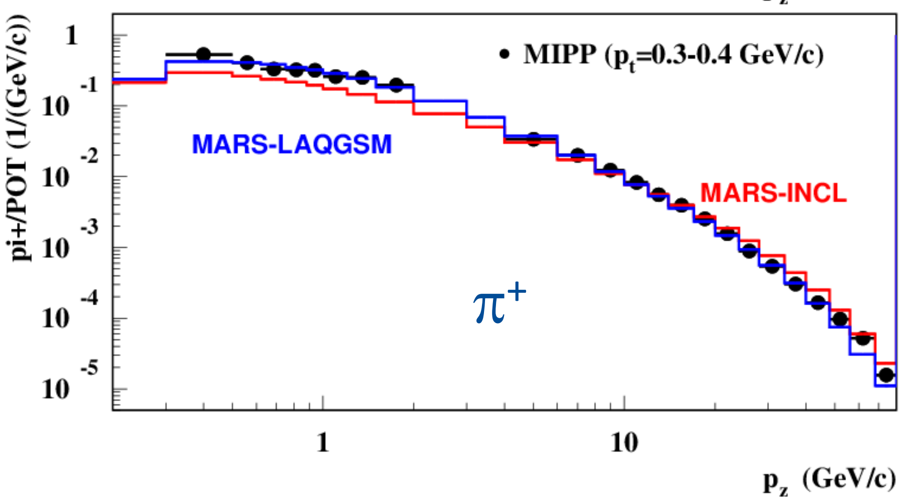




MARS Pion Spectra *vs* MIPP Data at 120 GeV







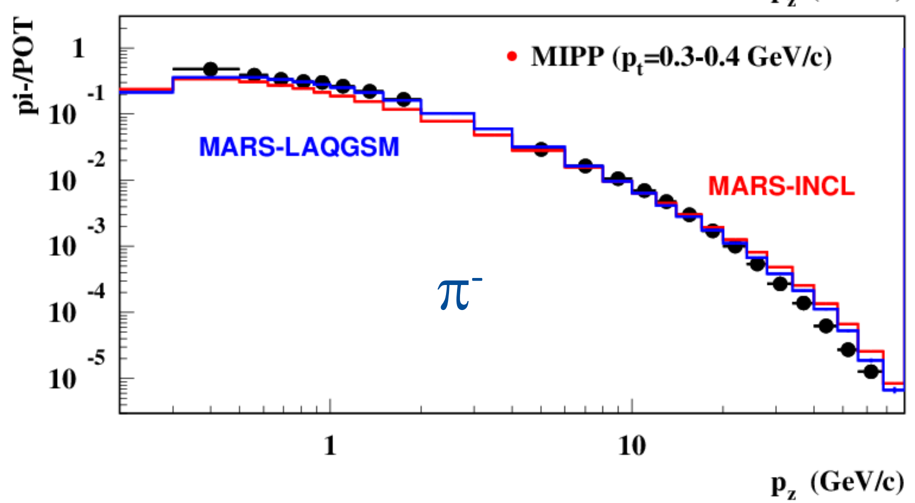
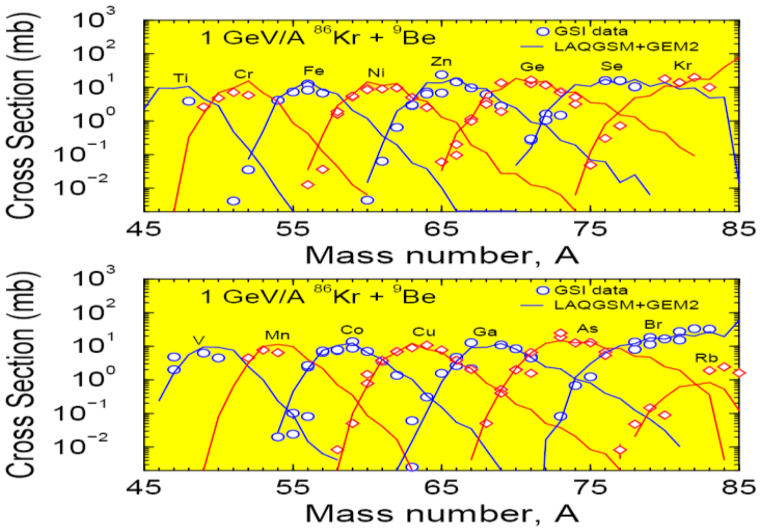
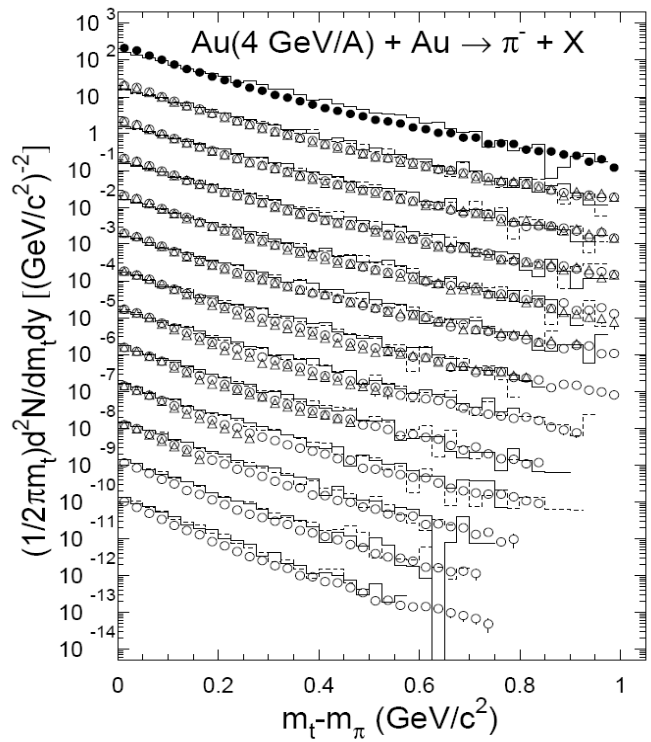
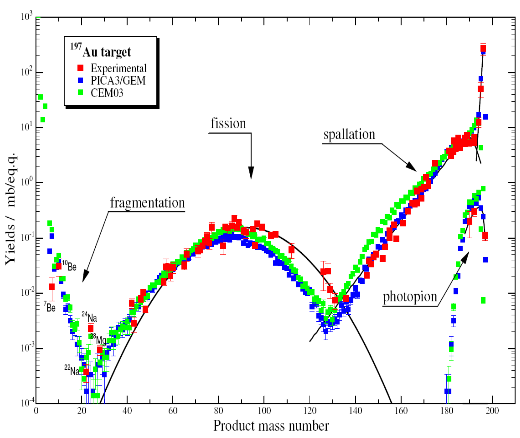


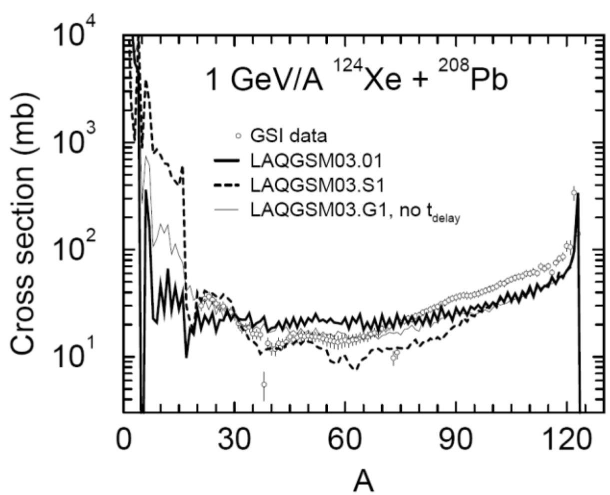
Photo-Nucleus and Nucleus-Nucleus





Bremsstrahlung (Emax=1 GeV) on gold





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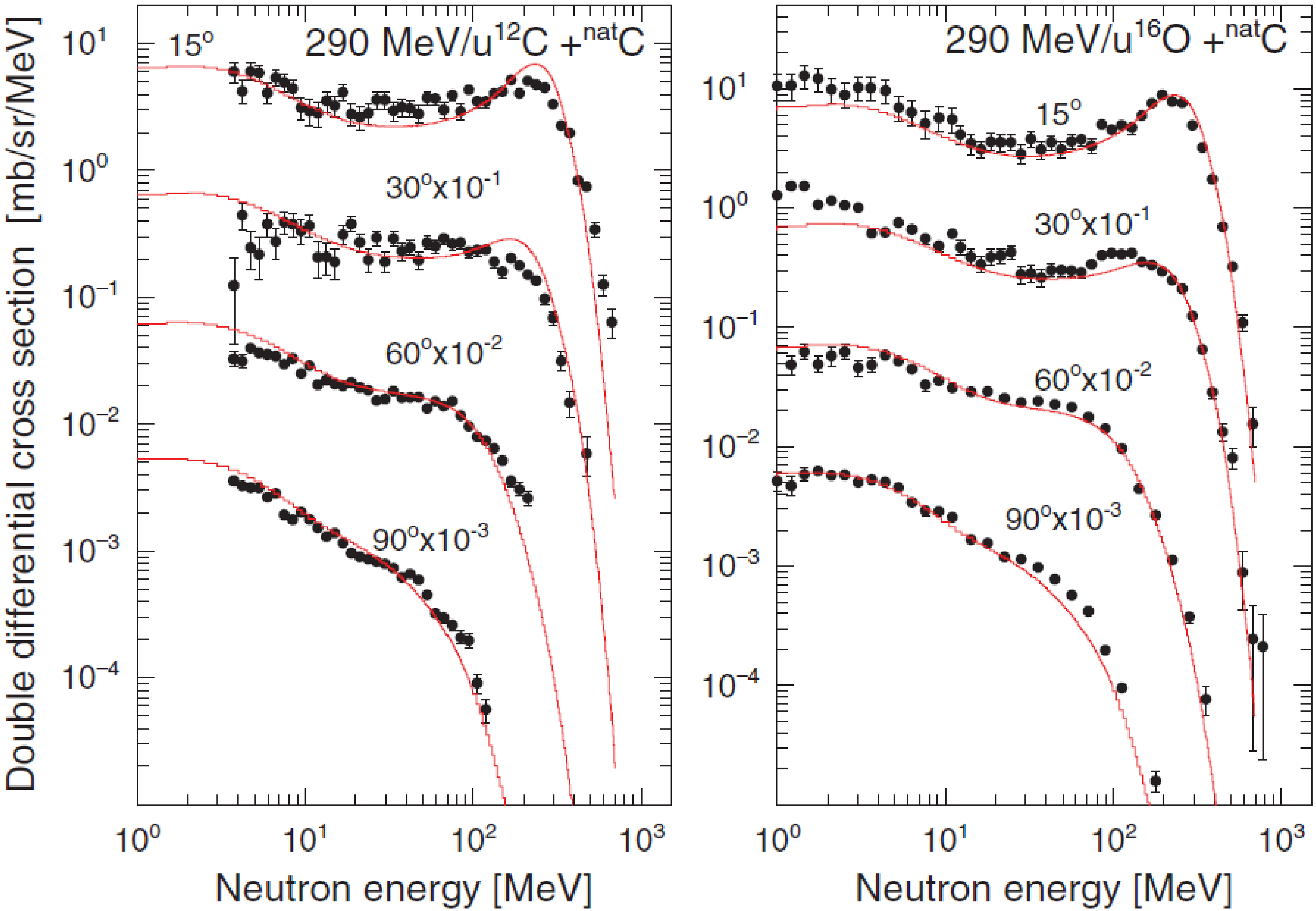
PHITS: 290 MeV/u ^{12}C and ^{16}O on ^{nat}C

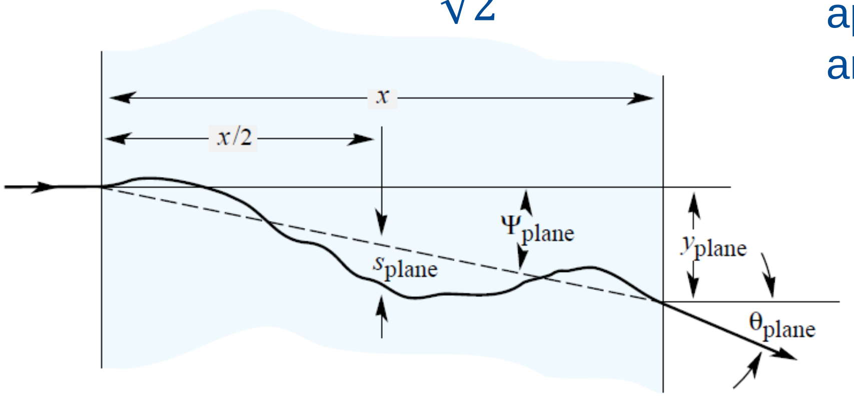


Quasi-Continuous Effects

To account for quasi-continuous effects in MCM, the charged particle path-length x between its starting point and the next discrete interaction point or a boundary to the nearest adjacent physical region or a point of leakage from the absorber is subdivided into **steps** ***s*** such that at every step the following conditions are fulfilled (*in the simplest approach*):

1. CSDA ionization energy loss $\Delta E = abs\left(\frac{dE}{dx}\right) \times s$ is small ($\frac{\Delta E}{E} \sim 1 - 5\%$)
2. Angle due to Multiple Coulomb scattering is small ($\theta_{plane} \leq \sim 0.1$ mrad)

$$\theta_0 = \theta_{plane}^{rms} = \frac{1}{\sqrt{2}}\theta_{space}^{rms}$$



It is sufficient for many applications to use a Gaussian approximation for the central 98% of the projected angular distribution with an RMS given by:

$$\theta_0 = \frac{0.0136 GeV}{\beta p} z \sqrt{\frac{x}{X_0}} [1 + 0.038 \ln(x\, z^2 / X_0 \beta^2)]$$

where z, β and p are the particle charge number, velocity and momentum and X_0 is the medium radiation length

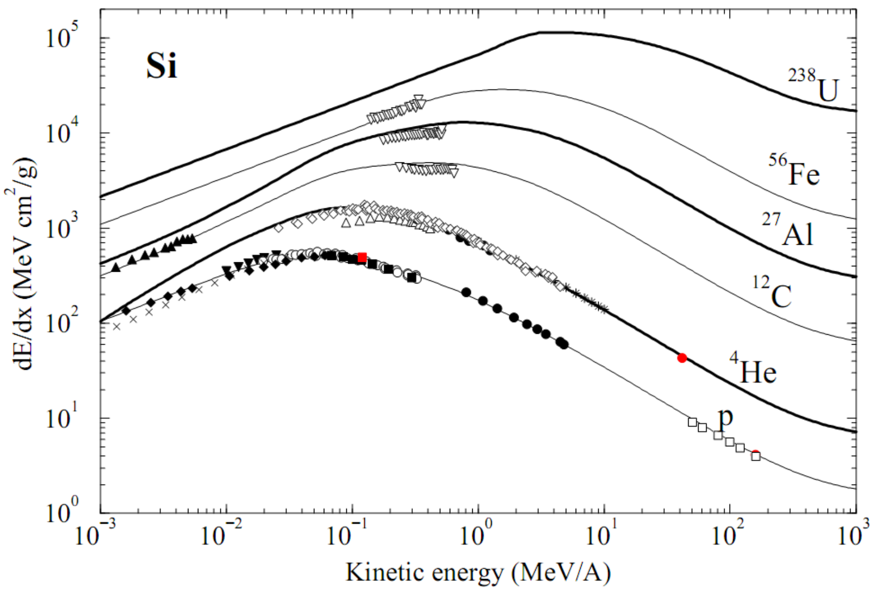
Mean CSDA Stopping Power

$$-\frac{1}{\rho}\frac{dE}{dx} = 4\pi N_A r_e^2 m_e c^2 z^2 \frac{Z}{A}\frac{1}{\beta^2}L(\beta)$$

$$L(\beta) = L_0(\beta) + \sum_i \Delta L_i$$

$$L_0(\beta) = \ln\left(\frac{2m_e c^2\beta^2\gamma^2}{I}\right) - \beta^2 - \frac{\delta}{2}$$

Bethe-Bloch formula



ΔLi: (i) **Lindhard-Sørensen** correction (exact solution to the Dirac equation; terms higher than z^2);

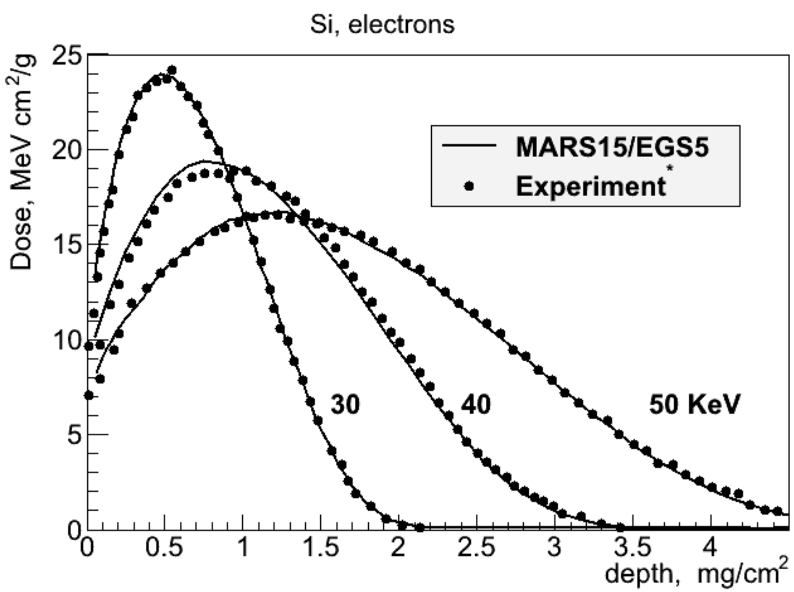
(ii) **Barkas** correction (target polarization effects due to low-energy distant collisions);

(iii) **shell** correction;

Projectile **effective charge** comes separately as a multiplicative factor that takes into account electron capture at low projectile energies (e.g., z_{eff} ~ 20 for 1-MeV/A ^{238}U in Al, instead of bare charge of 92).

Energy Loss and Energy Deposition Modeling

1. The CSDA dE/dx is widely used in quick estimations of energy loss by particle beams and in simplified simulations of energy loss and energy deposition along the charged particle tracks in hadronic and electromagnetic cascades.
2. In a more sophisticated approach used these days in several codes, precise modeling of knock-on electron production with energy-angle correlations taken into account is done for electronic losses.



3. Radiative processes – bremsstrahlung, pair production and inelastic nuclear interactions (via virtual photon) – for muons and high-energy hadrons - are modelled exclusively using pointwise x-sections.

Items (2) and (3) allow precise calculation of 3D energy deposition maps induced by high energy cascades.

Modelling in the State-of-the-Art MC Codes

- The radiative processes for high-energy muons and charged hadrons (direct e^+e^- pair production, bremsstrahlung and nuclear interaction *via* a virtual photon) as well as large $\frac{\Delta E}{E}$ ionization energy losses in “hard” collisions (see next slide) are modelled as discrete interactions.
- The large-angle (“Moliere”) Coulomb scattering is modelled via sophisticated algorithms, in some cases with energy-angle correlations taken into account.
- Customized steppers (*e.g.*, 8th order Runge-Kutta solver) are used for charged particle tracking in complex geometry with complex magnetic and electric fields.
- Decays of unstable charged and neutral particles are modelled on a step either analogously or with one of the variance reduction techniques (modified decay length or forced decays).

Monte-Carlo Simulation Scheme

The particles produced at the discrete interaction vertex are placed to the history bank, with one of them taken for the further transport to a new interaction point using the same techniques described in the previous slides. It is done with allowance for the particular features of the system (complex geometry, nonuniform material distribution, composite materials), decay of unstable particles, the possible quasi-continuous effects of the electromagnetic processes (ionization and radiative energy loss and multiple Coulomb scattering) and impact of magnetic and electric fields.

Virtually any functional of the random quantities ξ can be found directly during the simulation. The simulation of the history ends when the bank is empty and all the particles are absorbed or emitted from the system. The simulation is then repeated N times until the required statistical accuracy of the functionals is reached.

Response of Additive Detector

If the differential flux density is known, the reading (response) of any additive detector (in the broad sense) can be represented as

$$Res(t) = \iiint D\left(\vec{r}, \overrightarrow{\Omega}, E, t\right) \Phi\left(\vec{r}, \overrightarrow{\Omega}, E, t\right) d\vec{r}\, d\overrightarrow{\Omega}\, dE \qquad (1)$$

where $D\left(\vec{r}, \overrightarrow{\Omega}, E, t\right)$ is the sensitivity function of the detector, e.g., a light yield in scintillator. This is the average contribution to the detector readings from a unit path length of the particle with the coordinates $\left(\vec{r}, \overrightarrow{\Omega}, E, t\right)$ in the detector volume. Hence, the ***alternative definition of the differential flux density*** (with $D(\boldsymbol{x}) = 1$) as a quotient of the sum of the particle track length segments dl_k in the spatial volume dV of a phase volume near a phase point $\boldsymbol{x} = \left(\vec{r}, \overrightarrow{\Omega}, E, t\right)$ is $\Phi(\boldsymbol{x}) = \sum_k dl_k\, / dV$. Related ***energy deposition*** (with $D(\boldsymbol{x}) = dE$) for charged particles in dV is $\varepsilon\,(\boldsymbol{x}) = \sum_k dE_k dl_k\, / dV$.

Both are ready for prompt use in Monte-Carlo ***<u>track length estimate.</u>***

Atomic Displacement Cross-Section and NIEL

- Atomic displacement cross section

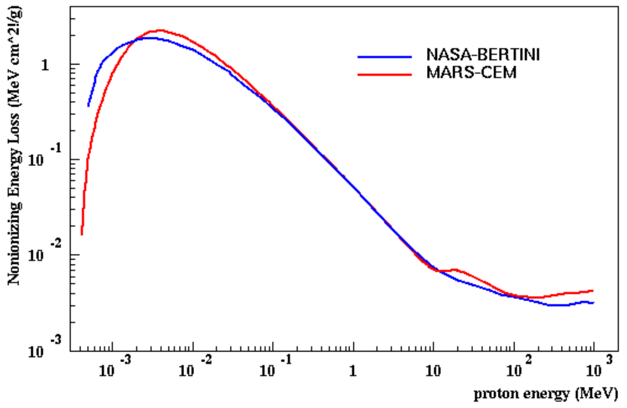
$$\sigma_d = \sum_r \int_{E_d}^{T_r^{\max}} \frac{d\sigma(E, Z_t, A_t, Z_r, A_r)}{dT_r} N_d(T_r, Z_t, A_t, Z_r, A_r) dT_r \qquad (2)$$

- *N_d* – number of stable defects produced, *E_d*–displacement threshold, *$d\sigma/dT_r$* - recoil fragment energy (*T_r*) distribution

- Non-ionizing energy loss (NIEL)

$$\left.\frac{dE}{dx}\right._{ni} = N \sum_r \int_{E_d}^{T_r^{\max}} \frac{d\sigma(E, Z_t, A_t, Z_r, A_r)}{dT_r} T_d(T_r, Z_t, A_t, Z_r, A_r) dT_r \qquad (3)$$

N – number of atoms per unit volume
T_d - damage energy=total energy lost in non-ionizing process (atomic motion)



Fermilab

Atomic Displacements (DPA) in MARS15

- Atomic displacement cross-section σ_{DPA} (2) is a reference way to characterize the radiation damage induced by neutrons and charged particles in crystalline materials. To evaluate a number of displaced atoms, Norget, Torrens and Robinson proposed in 1975 a standard (so-called, NRT-DPA), which has been widely used since. DPA is the left side of Eq. (1) while $D = \Sigma_{DPA}$ in the right side of Eq. (1).

- Energy of recoil fragments and new charge particles in (elastic and inelastic) nuclear interactions is used to calculate atomic displacement cross sections σ_{DPA} for the NRT model – w/o or with Nordlund/Stoller damage efficiency ξ(T) – for a number of stable defects

- Atomic screening parameters are calculated using the Hartree-Fock form-factors and recently suggested corrections to the Born approximation

- NJOY2016+ENDF/B-VIII.0(2018) is used to generate an NRT/Nordlund/Stoller database for 490 nuclides for neutrons from 10^{-5} eV to 200 MeV; DPA in neutron-nuclear interactions above 200 MeV are treated the same way as described in the second bullet

NRT "Standard" Model to Calculate a Number of Frenkel Pairs and Damage Energy

M.J. Norgett, M.T. Robinson, I.M. Torrens Nucl. Eng. Des 33, 50 (1975)

$$N_d = \frac{0.8}{2E_d} T_d$$

$$T_d = \frac{T_r}{1 + k(Z_t, A_t, Z_r, A_r) g(T_r, Z_t, A_t, Z_r, A_r)}$$

T_r, Z_r, A_r - recoil fragment energy=primary knock-on (PKA) energy, charge and atomic mass

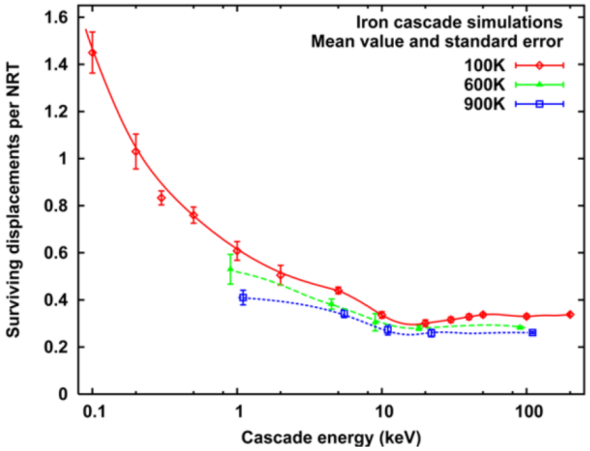
Z_t, A_t - charge and atomic mass of irradiated material

Nuclear physics (T_r, T_d) + solid state physics (N_d)

NRT-DPA is successfully applied to correlate data from many studies involving direct comparison from different irradiation environments

Efficiency Function (1): Stoller MD Parametrization

Corrections to NRT to account for atom recombination in elastic cascading. Database based on MD simulations. Its parametrization, efficiency function $\xi(T)=N_D/N_{NRT}$, is used for several years in MARS15 (=1 if >1, since 2016).



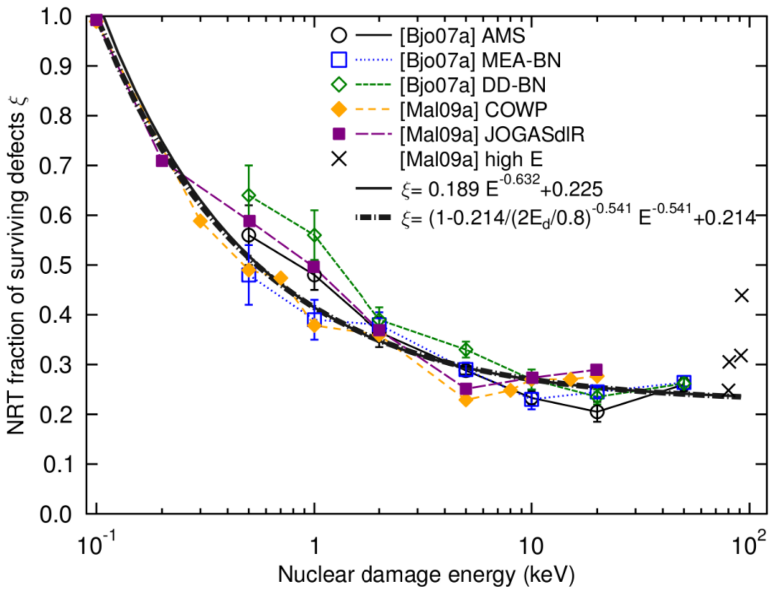
<u>Temperature dependence.</u> The calculations of Stoller (J. Nucl.Mater. 276 (2000) 22) for iron at 100-900K show some temperature dependence of the number of stable defects. At the same time the comparison of displacement cross-sections for p+Fe calculated using Stoller defect generation efficiency with the displacement cross-sections derived by Jung (J. Nucl. Mater. 117 (1983) 70) from low temperature experiments shows very good agreement.

Efficiency Function (2): Nordlund ARC-DPA

Nordlund's the ARC-DPA concept (athermal recombination-corrected DPA, in MARS15 since 2016):

"The recombination process does not require any thermally activated defect migration (atom motion is caused primarily by the high kinetic energy introduced by the recoil atom), this recombination is called "athermal" (i.e. it would also happen if the ambient temperature of the sample would be 0 K)."

"**<u>The arc-dpa concept allows empirical validation against frozen defects at cryogenic temperature</u>** (whereas NRT is an unobservable quantity)."



Modified NRT

$$N_d = \begin{cases} 0 & T_d < E_d \\ 1 & E_d < T_d < 2.5E_d \\ \dfrac{T_d}{2.5E_d}\xi(T_d) & 2.5E_d < T_d \end{cases}$$

with efficiency function

$$\xi(T) = 0.214 + 0.786 \times (2.5E_d / T)^{0.541}$$

Experimental Data Relevant to DPA Analysis

Jung et al, Greene et al and Iwamoto measured electrical resistivity change due to protons, electrons, light ions, fast and low-energy neutrons at low temperatures and low doses. It is connected to displacement cross section σ_d

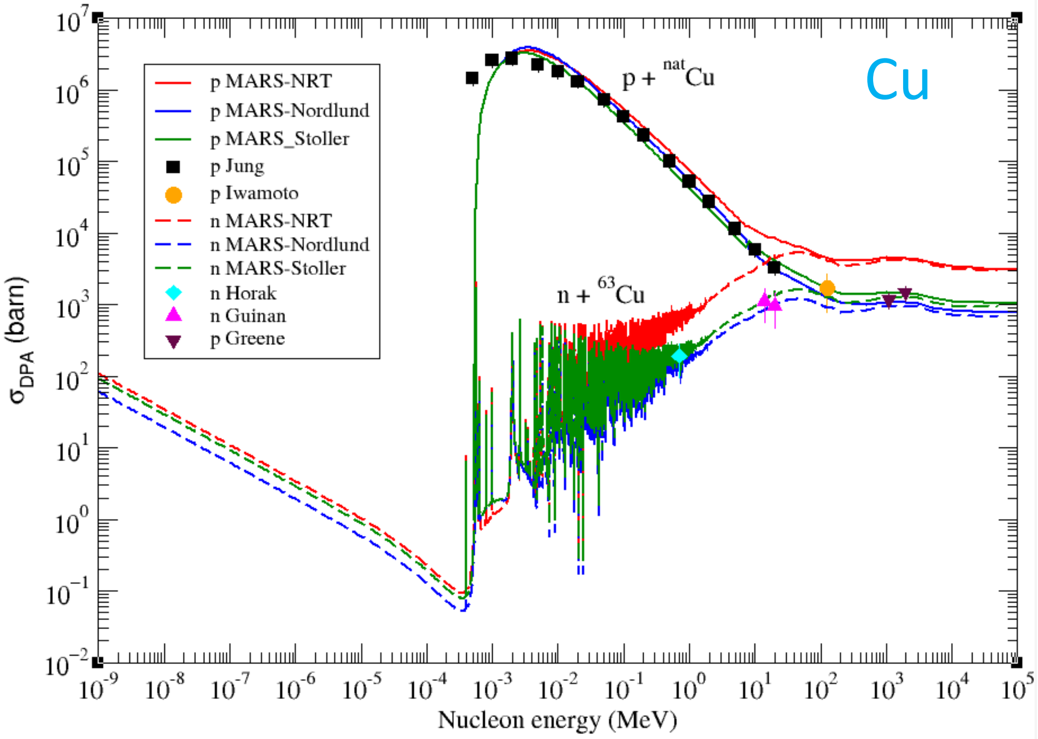
$$\Delta\rho_d(\Phi, E) = \Phi\ \sigma_d(E)\rho_F$$

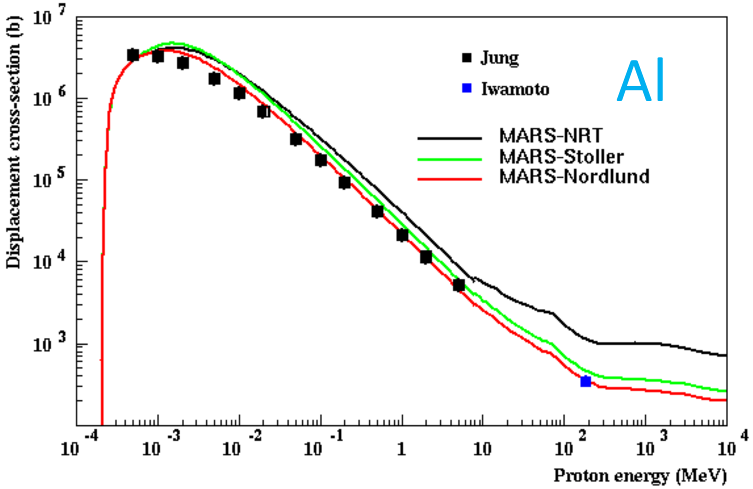
ρ_F is a resistivity per unit concentration of Frenkel defects. This constant cannot be accurately calculated and is determined from measurements. Jung and Greene groups choose different ρ_F (μΩm/u.c.) for the same material

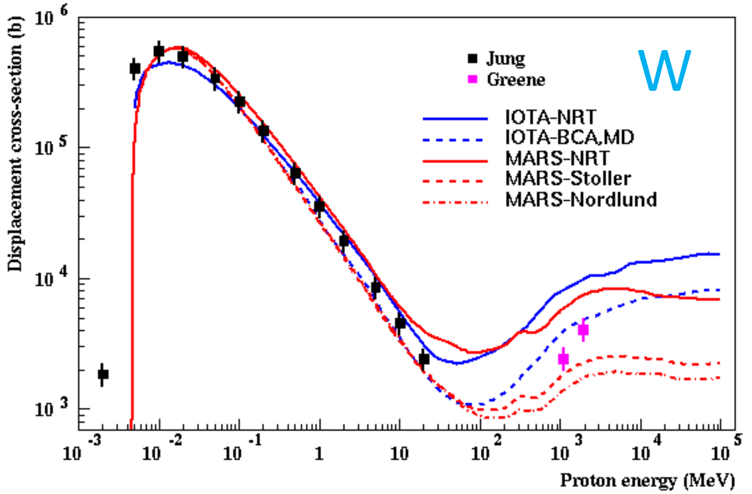
	Jung	Greene	Iwamoto
Cu	2.5 ± 0.3	2	2 ± 1
W	27 ± 6	14	-

Konobeev, Broeders and Fisher (IOTA) note that Greene's choice for W seems questionable taking into account later analysis

Proton and Neutron DPA Verification







DPA in FLUKA

Charged particles and heavy ions

- During transport: The restricted non-ionizing energy loss (3)
- Below threshold: The integrated nuclear stopping power with Lindhard partition
- At elastic and inelastic interactions: Transported and treated as “below threshold”

Neutrons

- High energy E>20 MeV: treat recoils after interaction as a “normal” charged particle/ion
- Low energy E≤20 MeV (group-wise): NIEL from NJOY
- Low energy E≤20 MeV (point-wise): treat recoil (if created) as a “normal” charged particle/ion

Results are close to those of MARS15

FLUKA (www.fluka.org)

FLUKA is a general-purpose particle interaction and transport (**Fortran 77**) code. It comprises all features needed for radiation protection, such as detailed hadronic and nuclear interaction models up to 10 PeV, full coupling between hadronic and electromagnetic processes and numerous variance reduction options. The latter include weight windows, region importance biasing, and leading particle, interaction, and decay length biasing (among others).

The capabilities of FLUKA are very good for studies of induced radioactivity, especially with regard to nuclide production, decay, and transport of residual radiation (cite from RPP). In particular, particle cascades by prompt and residual radiation are simulated in parallel based on the microscopic models for nuclide production and a solution of the Bateman equations for activity build-up and decay. **FLUKA is *de facto* the official code in numerous LHC and other applications at CERN.**

FLUKA's Features (1)

The highest priority in the design and development of FLUKA has always been the implementation and improvement of sound and modern physical models. Microscopic models are adopted whenever possible, consistency among all the reaction steps and/or reaction types is ensured, conservation laws are enforced at each step, results are checked against experimental data at single interaction level.

As a result, final predictions are obtained with a minimal set of free parameters fixed for all energy/target/projectile combinations. Therefore results in complex cases, as well as properties and scaling laws, arise naturally from the underlying physical models, predictivity is provided where no experimental data are directly available, and correlations within interactions and among shower components are preserved.

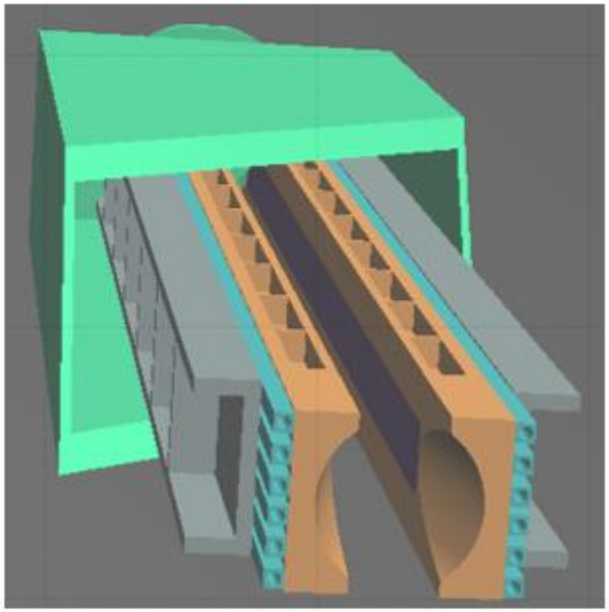
FLUKA's Features (2)

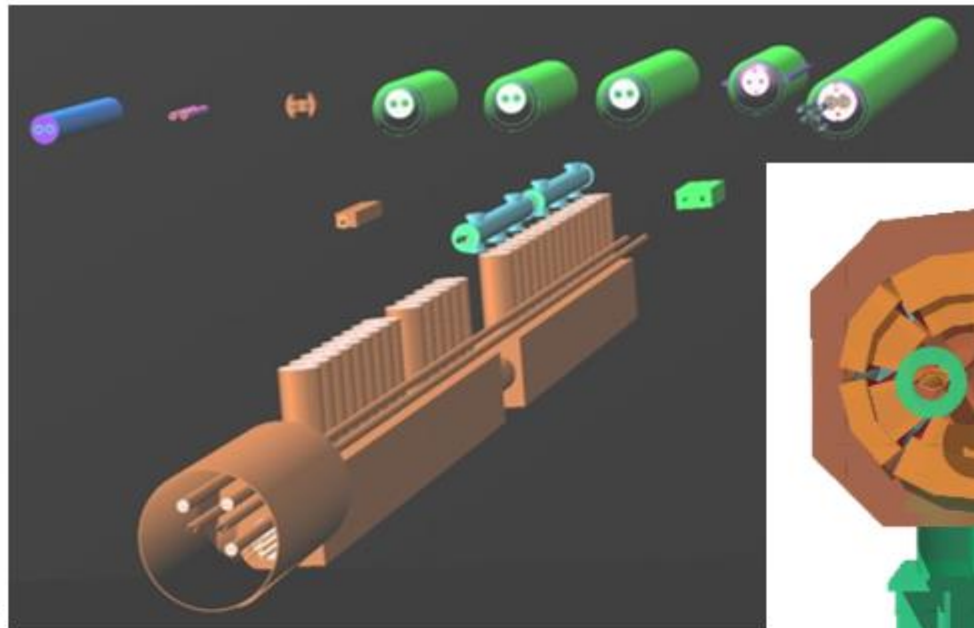
FLUKA can handle very complex geometries, using an improved version of the well-known Combinatorial Geometry (CG) package. The FLUKA CG has been designed to track correctly also charged particles (even in the presence of magnetic or electric fields). Various visualisation and debugging tools are also available.

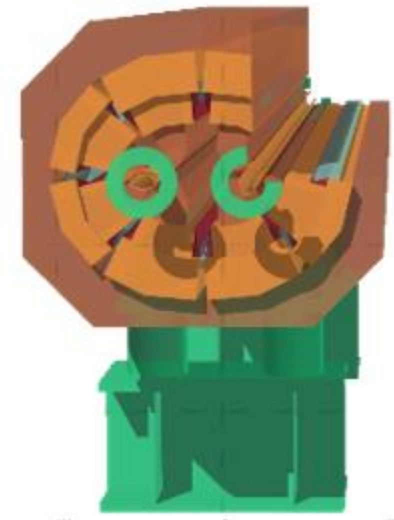
Similar to the MARS15 code, FLUKA has a double capability to be used in a biased mode as well as a fully analogue code. That means that while it can be used to predict fluctuations, signal coincidences and other correlated events, a wide choice of statistical techniques are also available to investigate punch-through or other rare events in connection with attenuations by many orders of magnitude.

FLUKA Geometry Modeling (1)

NEED FOR DETAILED MODELS OF ACCELERATOR COMPONENTS WITH ASSOCIATED SCORING





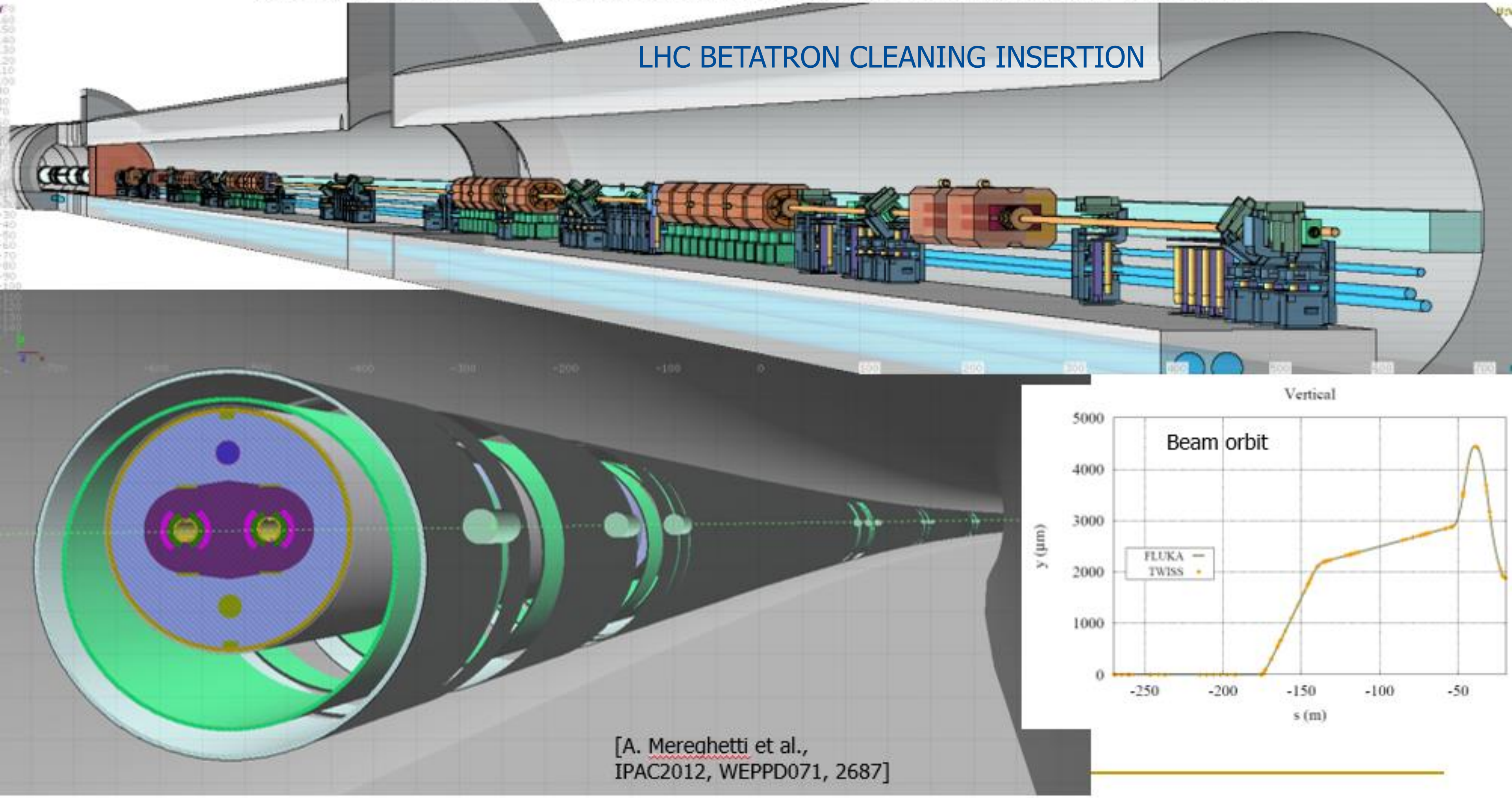


ELEMENT SEQUENCE AND RESPECTIVE MAGNETIC STRENGTHS
IN THE MACHINE OPTICS (TWISS) FILES

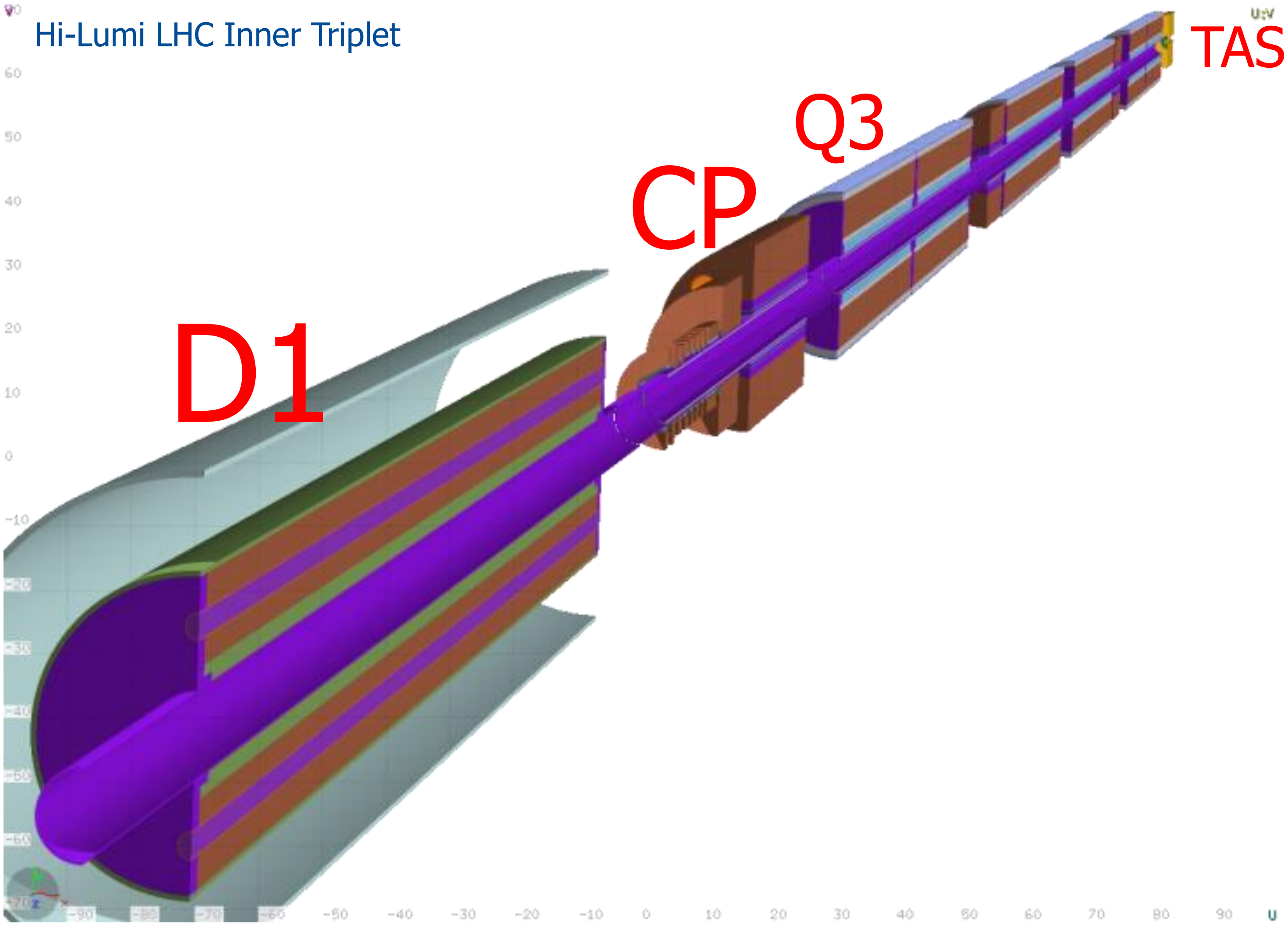
F. Cerutti

FLUKA Geometry Modeling (2)

Profiting from roto-translation directives and replication (lattice) capabilities,
the AUTOMATIC CONSTRUCTION OF COMPLEX BEAM LINES,
including collimator settings and element displacement (BLMs), is achievable



FLUKA Geometry Modeling (3)



F. Cerutti

GEANT4 (geant4.cern.ch)

GEANT4 is an **object-oriented toolkit** consisting of a kernel that provides the framework for particle transport, including tracking, geometry description, material specifications, management of events and interfaces to external graphics systems. The kernel also provides interfaces to physics processes. It allows the user to freely select the physics models that best serve the particular application needs. Implementations of interaction models exist over an extended range of energies, from optical photons and thermal neutrons to high-energy interactions required for the simulation of accelerator and cosmic ray experiments.

G4 is the industry standard for HEP detector simulation. To facilitate the use of variance reduction techniques, general-purpose biasing methods such as importance biasing, weight windows, and a weight cut-off method have been introduced directly into the toolkit. Other variance reduction methods, such as leading particle biasing for hadronic processes, come with the respective physics packages.

GEANT4 Physics Models

A comprehensive set of the well-established models comprises GEANT's physics lists for users to chose from. Substantial efforts were and still are put by the GEANT4 team on validation and verification of electro-magnetic physics in the code and hadronic physics loosely defined to cover any reaction which can produce hadrons in final state: purely hadronic interactions, lepton- and gamma-induced nuclear reactions, and radioactive decay.

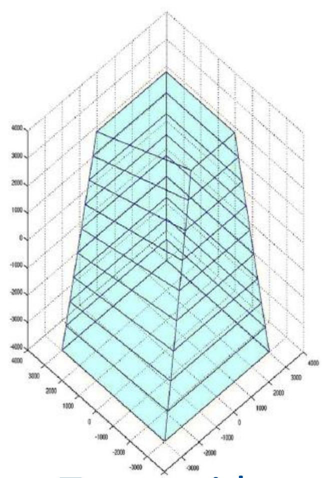
Models and x-sections are provided which span an energy range from sub-eV to TeV. Following the toolkit philosophy, more than one model or process is usually offered in any given energy range in order to provide alternative approaches for different applications.

GEANT4's performance was noticeably improved after several international benchmarking campaigns over last 15 years.

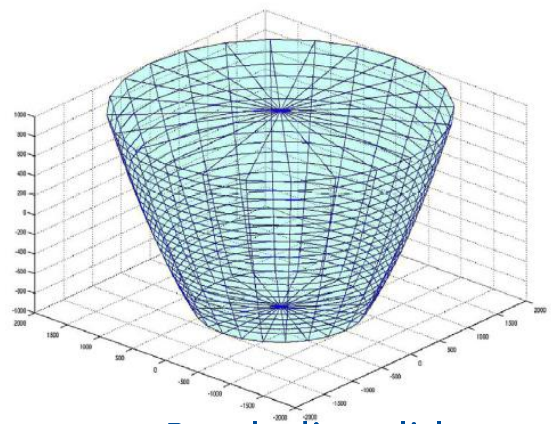
GEANT4 Geometry

There are several ways to build a geometry model in GEANT4. The standard one is to write a C++ code that contains all the definitions, material, dependence, position and hierarchy assignments, and arranges all these in the model. The shapes or geometrical primitives can be taken from a comprehensive library built in the toolkit. Fragments of the model can be imported and exported from external files according to two different formats: GDML or plain ASCII text (next slide).

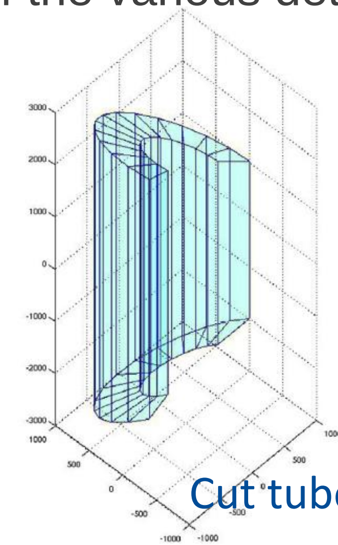
GEANT4 provides internal modules which allow the interpretation and conversion of these formats to and from the internal geometry representation, without the need for C++ programming for the implementation of the various detector description setups.



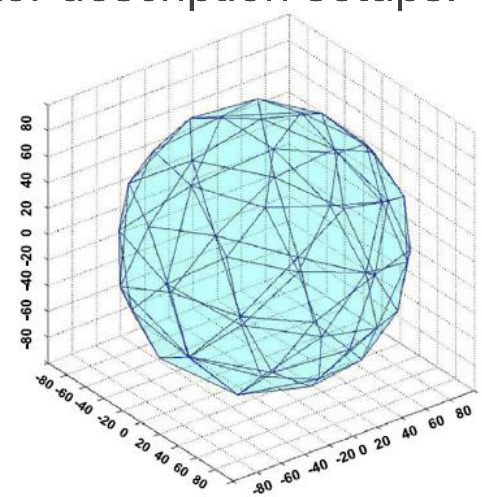
Trapezoid



Parabolic solid



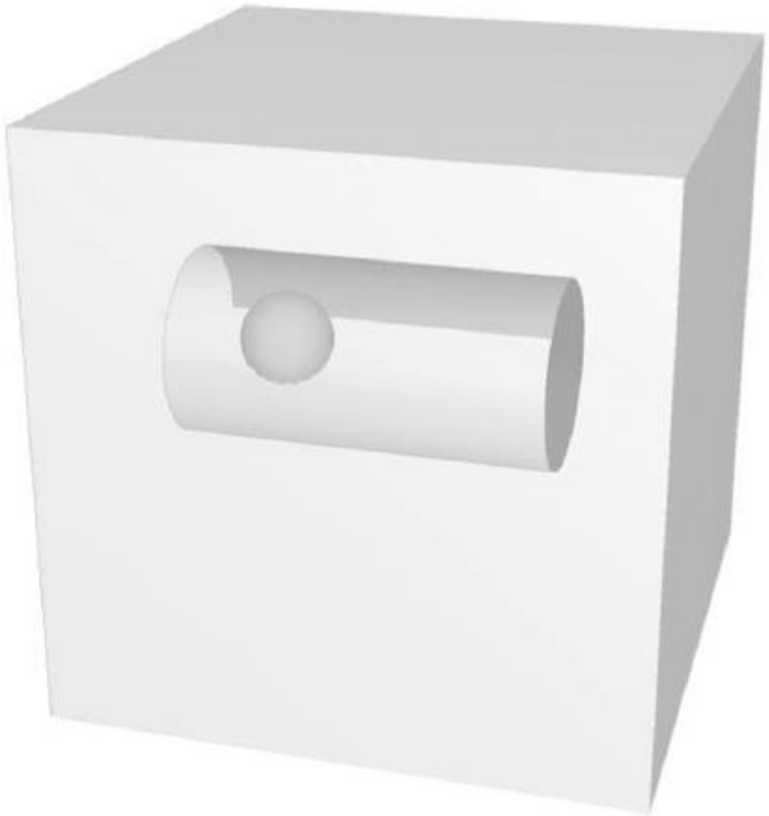
Cut tube



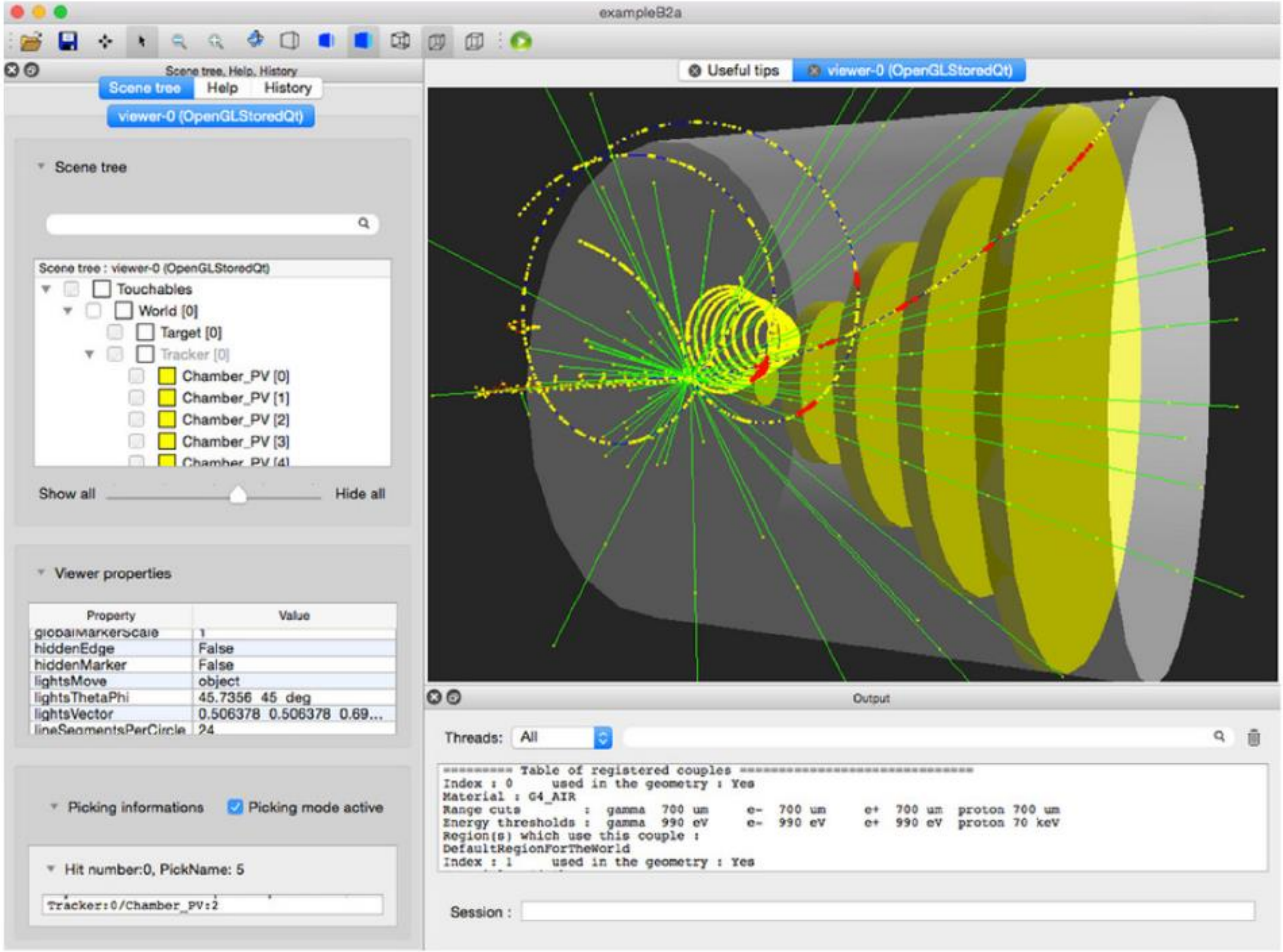
Sphere

GEANT4: Example of Geometry ASCII Text Format

```
// Define a parameter for later use
 :P DIMZ 5.

// Define materials
 :ELEM Hydrogen H 1. 1.
 :ELEM Oxygen O 8 16.
 :ELEM Nitrogen N 7 14.
 :MIXT Air 1.214E-03 2
    Nitrogen 0.75
    Oxygen 0.25

// Define rotation matrix
 :ROTM R00 0. 0. 0. // unit matrix

// Define volumes and place them
 :VOLU world BOX 30. 30. 30. Air

 :VOLU "my tube" TUBE 0. 10. $DIMZ*4 G4_WATER
 :PLACE "my tube" 1 world R00 0. 0. $DIMZ

 :VOLU sphere ORB 5. G4_AIR
 :PLACE sphere 1 "my tube" R00 0. 1. 10.
```

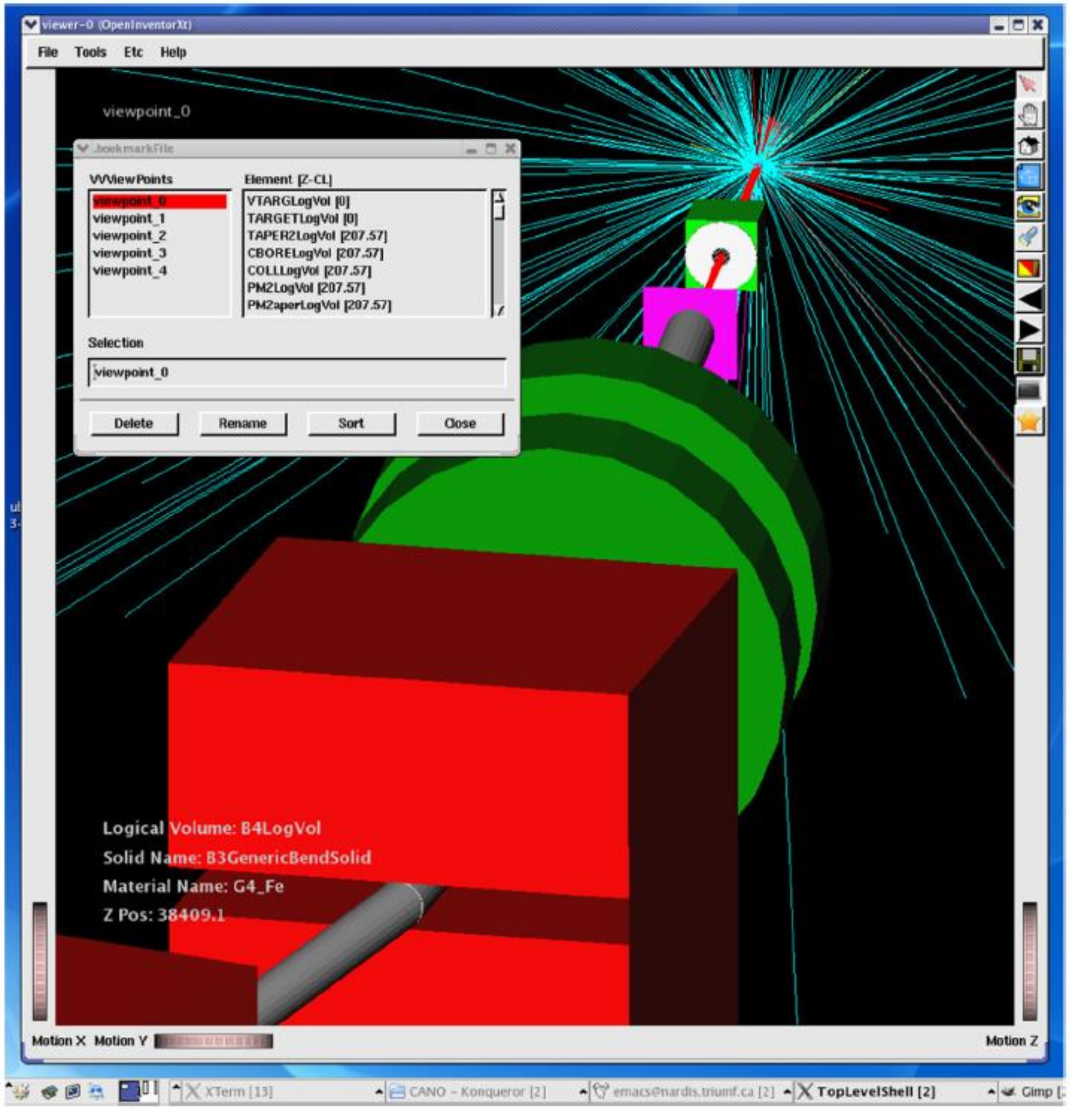


GEANT4: OpenGL Viewer Wrapped in Qt



Fermilab

GEANT4: Open Inventor Extended Viewer

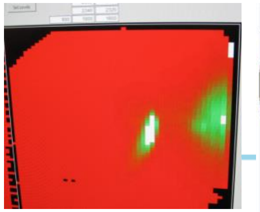
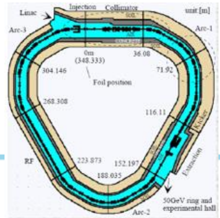
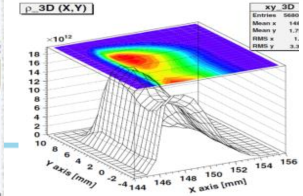
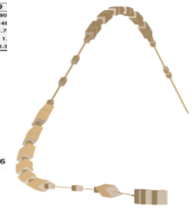
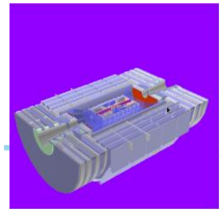
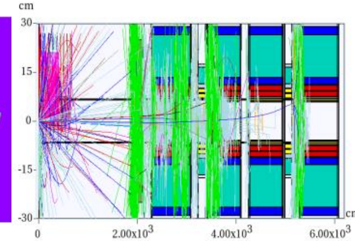
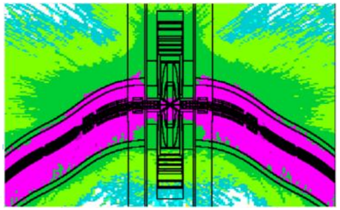


MARS Code System

The MARS code system is a set of Monte Carlo programs for detailed simulation of hadronic and electromagnetic cascades in an arbitrary geometry of shielding, accelerator, detector and spacecraft components with energy ranging from 10^{-5} electronvolt up to 100 TeV. It was originated by NM in 1974 at MEPhI (Moscow), and developed since at IHEP (Protvino), SSCL (Texas) and Fermilab.

Current MARS15 combines well established theoretical models for strong, weak and electromagnetic interactions of hadrons, heavy ions and leptons with a system which can contain millions of objects, ranging in dimensions from microns to hundreds kilometers in same setup. **Especially powerful in accelerator lattice, beamline and machine-detector interface applications.**

300 official users worldwide, tutorials, https://mars.fnal.gov

Particle yields:
p, n, π, K, μ, Σ, HI

Nuclide inventory

Radiation damage:
DPA, dose, H/He,
soft errors (SEE)

Detector background suppression

Beamline optimization,
beam loss, particle capture and collimation,
SC magnet quench

Prompt and residual radiation, shielding, impact on environment

Targetry: power dissipation, integrity (shock & buildup), magnetohydrodynamics

MARS15 Generic Features (1)

A setup can be made of up to 500 composite materials, with arbitrary 3-D magnetic and electric fields. Powerful user-friendly GUI is used for visualization of geometry, materials, fields, particle trajectories and results of calculations.

It has 6 geometry options including ROOT and MCNP ones, flexible histograming, can use as an input MAD optics files through a powerful MAD-MARS Beam Line Builder, various tagging, biasing and other variance reduction techniques.

Bilateral geometry model exchange (via GDML files) with Geant4).

It is interfaced with MADX-PTC, EGS5 and DPMJET, can be interfaced with ANSYS (thermal and stress), MESA/SPHINX (hydrodynamics), and FRONTIER (magneto-hydrodynamics).

MARS15 Generic Features (2)

- Customized steppers (with 8^{th} order Runge Kutta solver) for optimal particle tracking in SRF (with time-dependent electromagnetic fields and Dark Current production), quadrupole/dipole magnets and thick shielding
- Variance reduction techniques: multi-stage, splitting/Russian roulette, biasing, weight windows
- Verified set of flux-to-dose (FTD) conversion factors to calculate - in the course of Monte-Carlo - effective prompt dose distributions: ICRP103 + ICRP60+Cossairt(2009)+Pellicioni(2000) + MARS generated for neutrinos
- Nuclide production, decay, transmutation and calculation of the activity distribution is done with the built-in DeTra code
- MARS15 uses ENDF/B-VIII.0(2018) nuclear data to derive the NRT/Stoller/Nordlund DPA x-sections for neutrons from 10^{-11} to 200 MeV

MARS15: Exclusive, Inclusive and Hybrid

Most of the processes in MARS15, such as electromagnetic showers, hadron-nucleus interactions, decays of unstable particles, emission of synchrotron photons, photo-hadron production and muon pair production, can be treated exclusively (analogously), inclusively (with corresponding statistical weights), or in a mixed mode.

The choice of the mode is left for the user to decide, via the input settings.

Goal: Maximize computing efficiency $\varepsilon = t_0/t$, where t is CPU time needed to get a RMS error σ equal to the one in the reference method with CPU time t_0 provided $\sigma < 20\%$.

Fermilab

Material Description & Low-Energy Neutrons

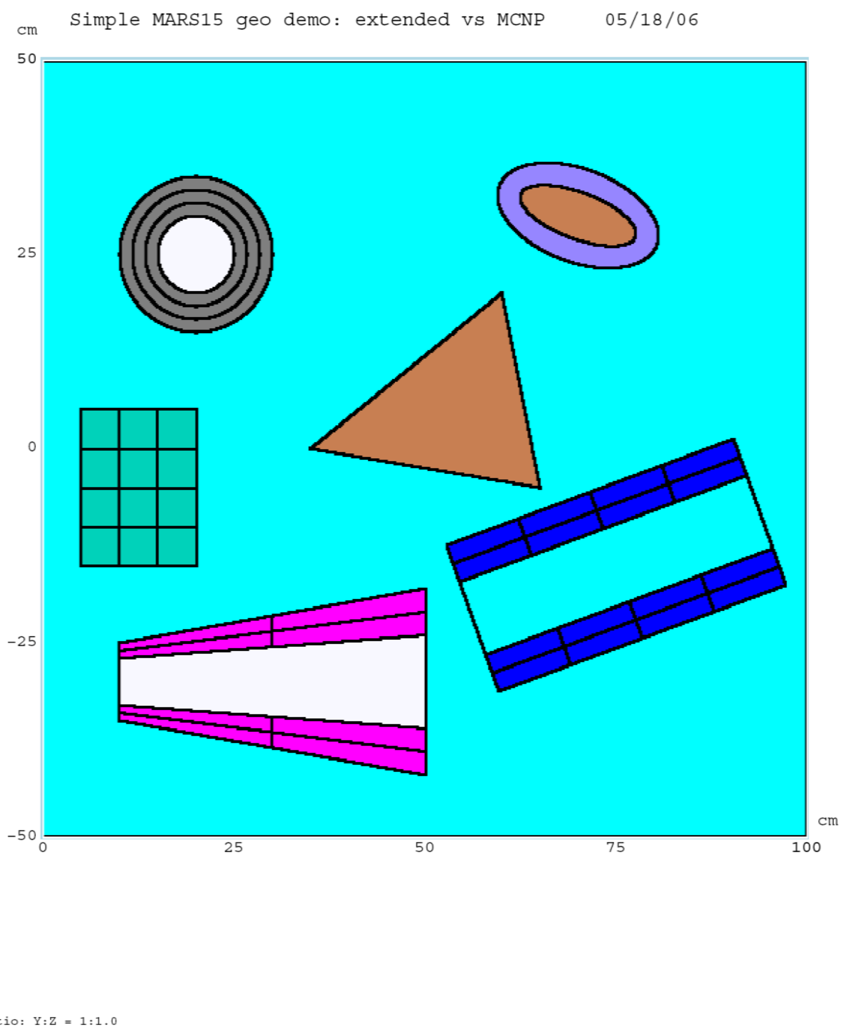
- The code automatically unpacks the elemental distributions into isotope distributions for both user-defined and those from the 176 built-in material definitions for use in the 10^{-11} MeV < E < 100 TeV energy range
- For neutron interactions at $10^{-11} < E_n < 14$ MeV, MARS15(2019) relies on the heavily validated and recently released library of ACE files based on ENDF/B-VIII.0(2018)
- There is no need anymore to add material description in the MCNP format after the STOP card in MARS.INP files: the code does automatically all the required interface work for every single isotope found in the given run
- Accurate treatment of material state (solid, liquid and gaseous); He^3 treatment

Geometry Description and ROOT-based Beamline Builder

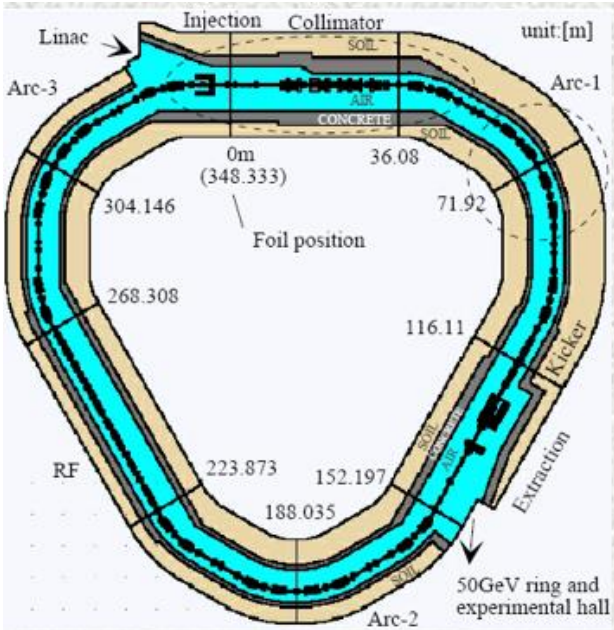
1. User-generated via MARS extended geometry input files
2. User-generated ROOT files: Quantum Leap!
3. GDML files (bilateral exchange with Geant4 teams)
4. G4beamline's BruitDeFond can generate MARS's input files MARS.INP, GEOM.INP and FIELD.INP
5. STEP files from project CAD models used to generate semi-automatically ROOT geometry modules
6. Lattice and beamline components such as dipole and quadrupole magnets, correctors, accelerating cavities, cryomodules and tunnel with all the details available on geometry, materials and electromagnetic fields by means of the advanced ROOT-based Beamline Builder

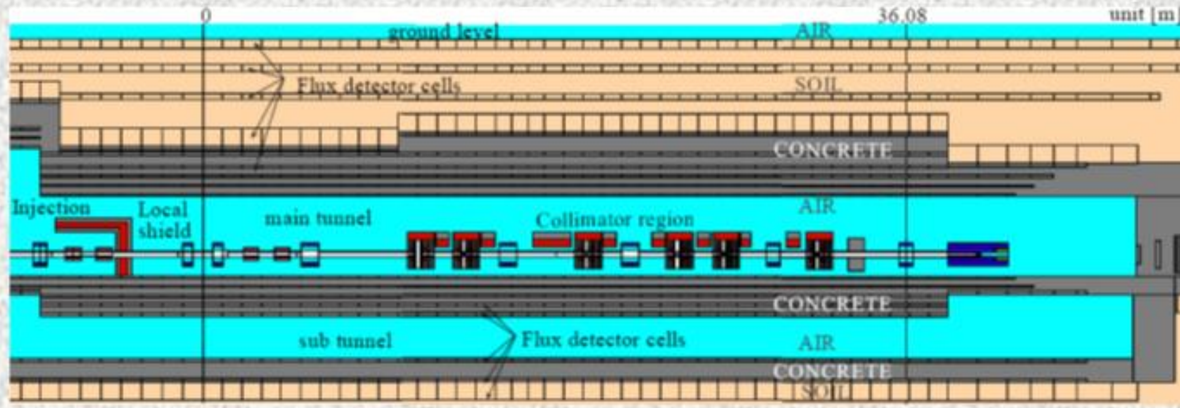
MARS15 Simple GEOM.INP Example

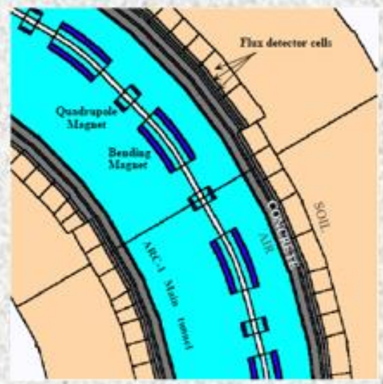
```
Extended Demo  05/17/06
OPT
box-1      1 0 2   0.  -5.   5.  10.  10. 15. 1 4 3
cyl-1a    -2 1 7   0.   0.   0.   0.   5. 20.
cyl-1a    -2 1 1   0.   0.   0.   5.  10. 20. 4 2
ball-a     3 0 8   0.   25. 20.   0.   5.
ball-b     3 0 3   0.   25. 20.   5.  10. 3
cone-in   -4 0 0   0. -30.  30.   0.   3.  0.  6. 20.
cone-out  -4 0 4   0. -30.  30.   3.   5.  6. 12. 20. 2 2
th         5 0 6   0. 0. 35. 5. 3. 55. 0. 20. 60. 0. -5. 65.
ell-tub1  -6 2 6   0.   0.   0.   8.   3.  0.  40.
ell-tub2  -6 2 5   0.   0.   0.   8.   3.  3.  40.
TR1  0.  -15. 75. -20.
TR2  0.   30. 70.  20. 90.
stop
```

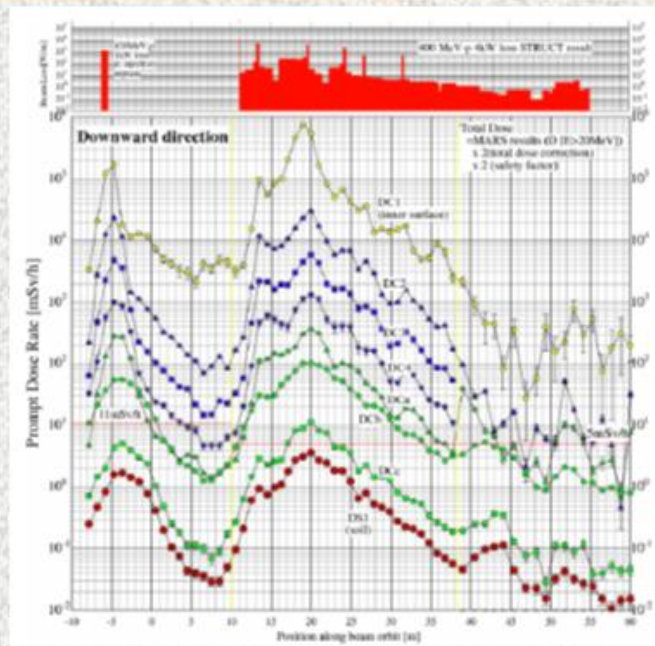


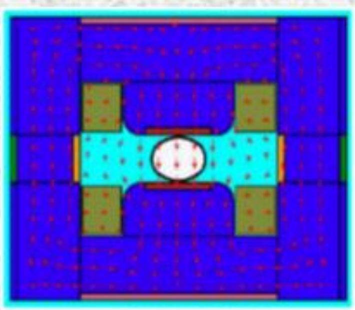
MMBLB Model: J-PARC 3-GeV Ring

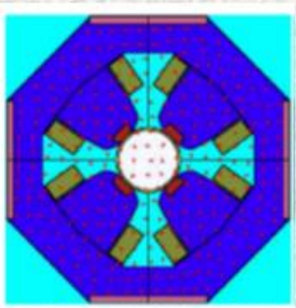












G4beamline's BruitDeFond Can Generate MARS's Input Files

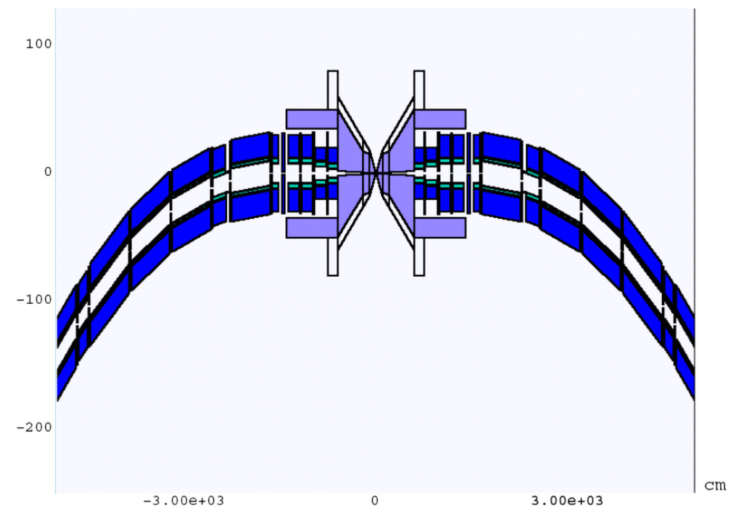
BruitDeFond **BeamMaker**

Tom Roberts

MARS.INP
GEOM.INP
FIELD.INP

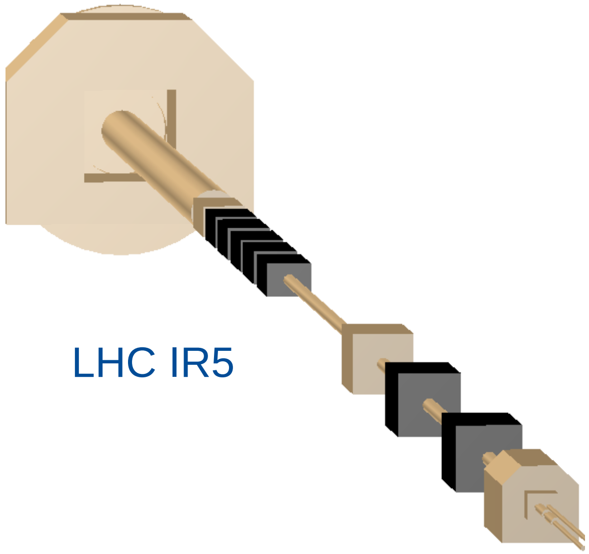
BeamMaker.txt

MARS15

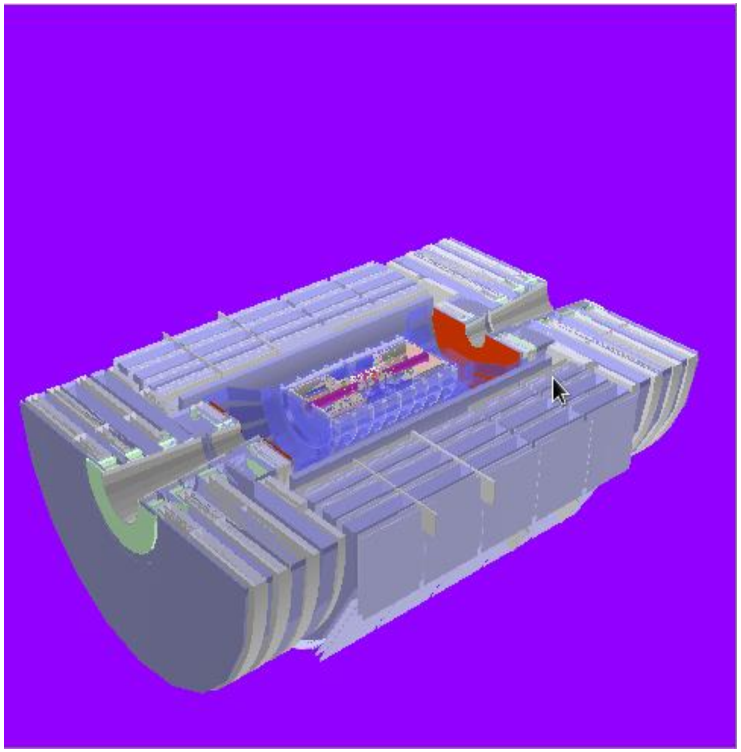


- *BruitDeFond* can generate MARS.INP and GEOM.INP files.
- The *extended* geometry is description is used.
- The field is described by the FIELD.INP file which is read by the MARS user subroutine "field" that we wrote.
- We use the same BeamMaker.txt file for the MARS input.

MARS15 ROOT-based Models



LHC IR5



LHC CMS detector

Fermilab Booster by ROOT-based BeamlineBuilder

MARS15 Generic Features (3)

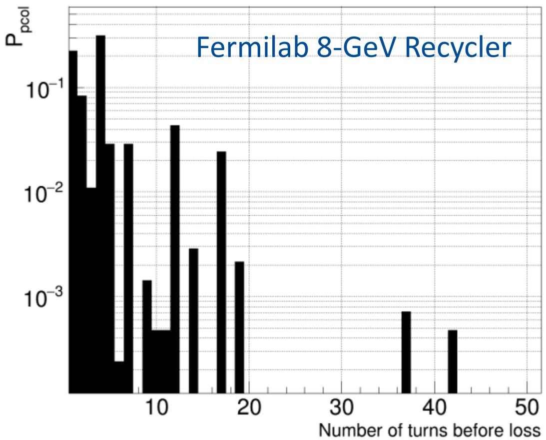
- A **tagging module** allows one to tag the origin of a given signal for source term or sensitivity analyses. Several variance reduction techniques, such as weight windows, particle splitting, and Russian roulette are possible.

- Beam-induced bulk damage in silicon detectors and electronics (via 1-MeV equivalent neutron fluence) and coming algorithm to model Single-Event Upset (SEU) or soft errors.

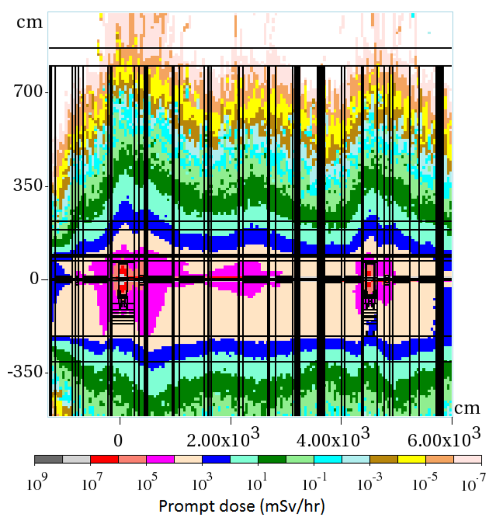
- ***The powerful capabilities of MARS15 for simulation in accelerator environment*** with the MARS-MAD Beamline Builder (**MMBLB**) working in concert with an accelerator tracking code (since almost 20 years ago) and with a recent active merge with MADX-PTC for a convenient creation of accelerator models and multi-turn tracking and cascade simulation in accelerator and beamline lattices.

- MARS15 is routinely used in concert with ANSYS for iterative studies of thermo-mechanical problems and can be interfaced to a hydrodynamic code to study phase transition and "**hydrodynamic tunneling**" – first done by SSC-LANL collaboration for a 20-TeV proton beam in 1993.

MARS-MADX-PTC: Fermilab Recycler and ILC

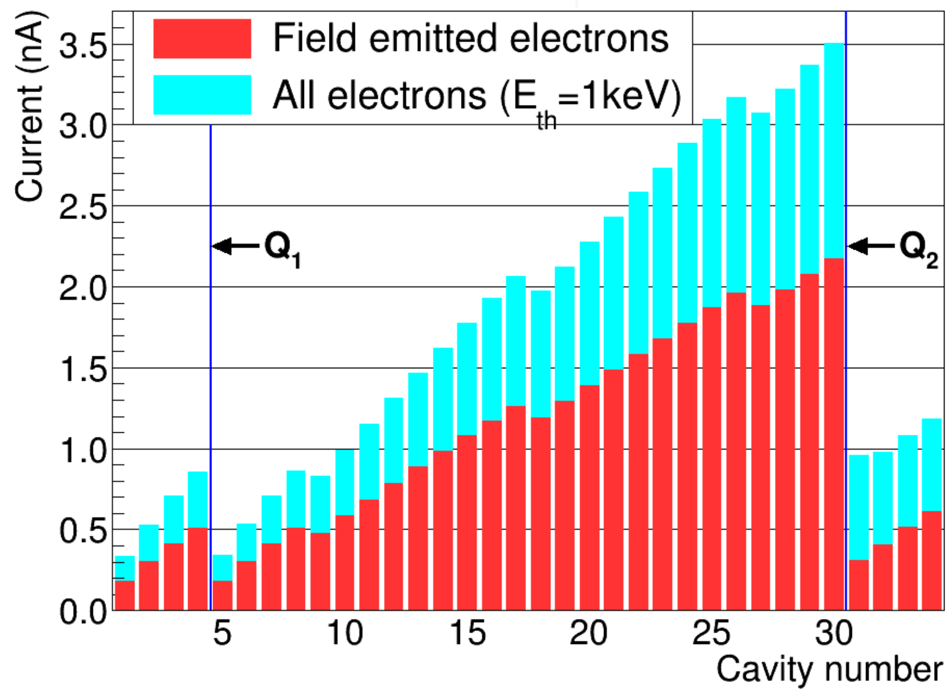


Probability to be lost for beam halo protons passed through the primary collimator vs #turns



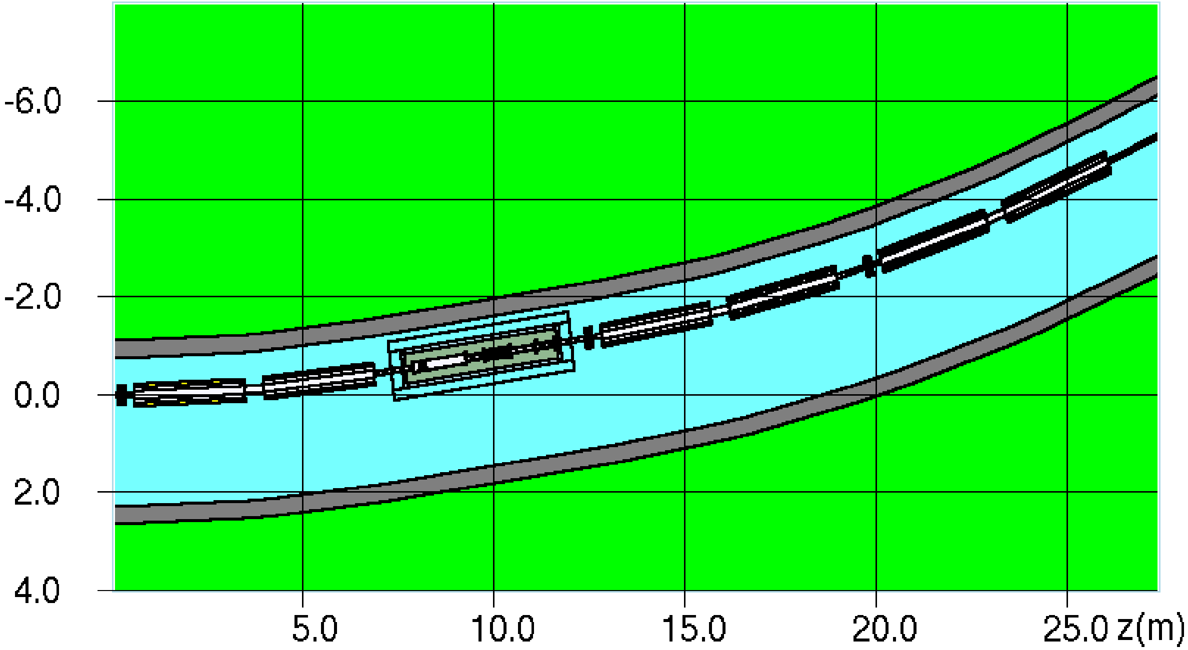
Prompt dose in collimation region

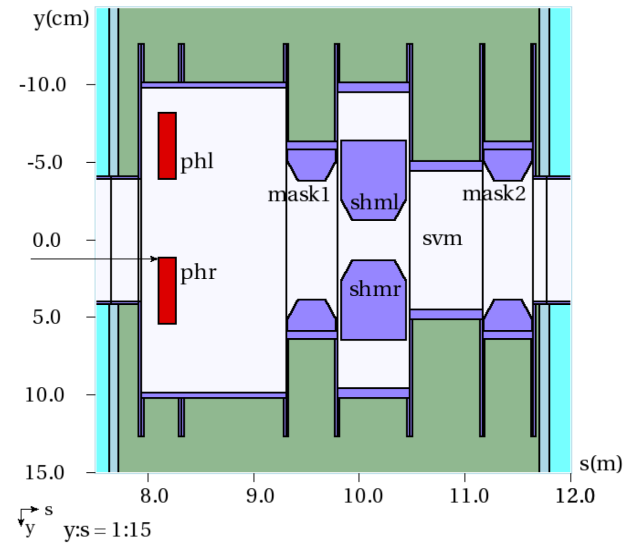
MARS15 SRF model (ILC & LCLS-II)

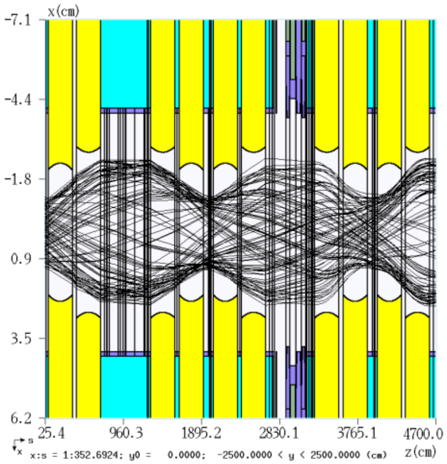


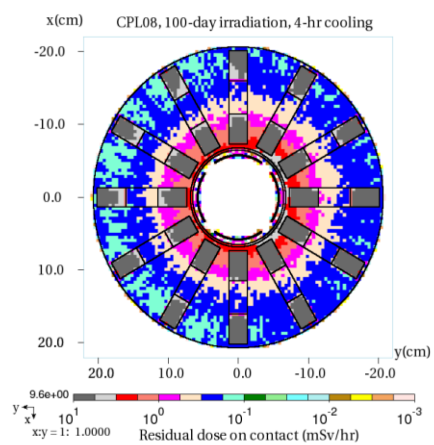
Dark current electrons and EMS electrons in ILC aperture with their loss responsible for radiation load to components and radiation field in ILC tunnel

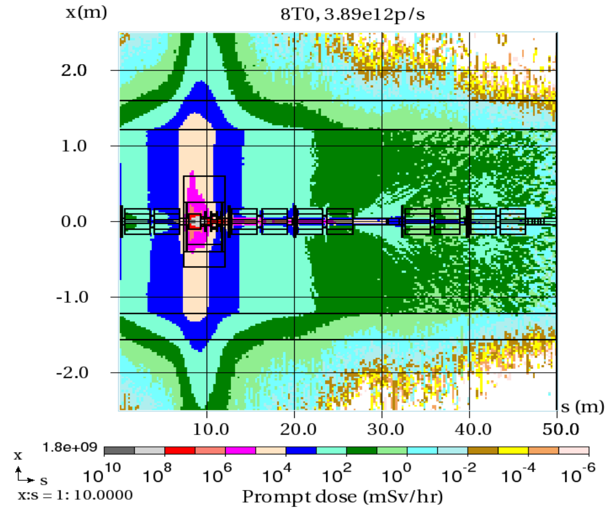
Booster New Collimation System











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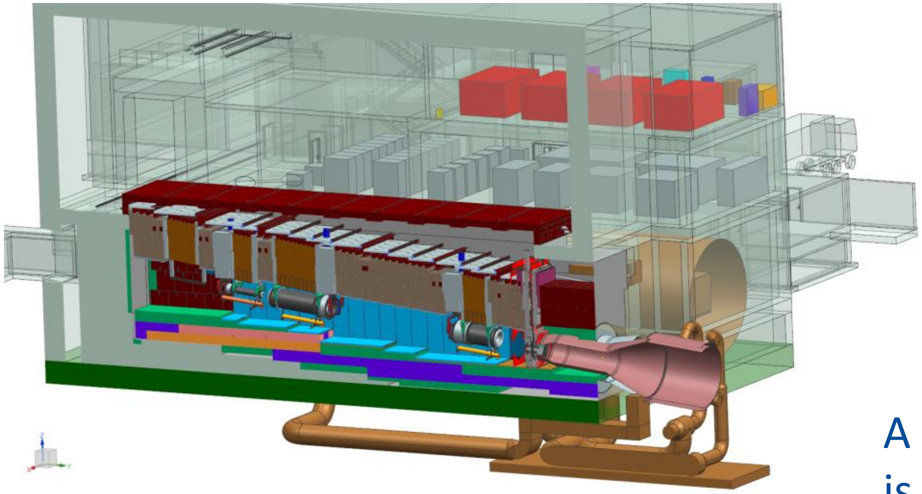
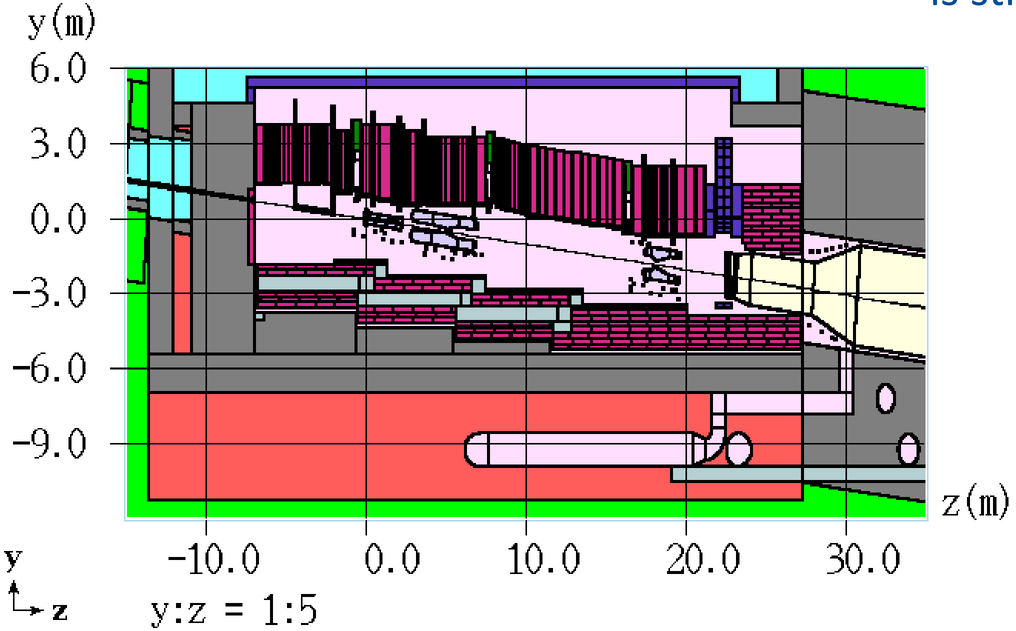
Target Station (TS): CAD & MARS15 Models



A replaceable target design is still in a preliminary stage



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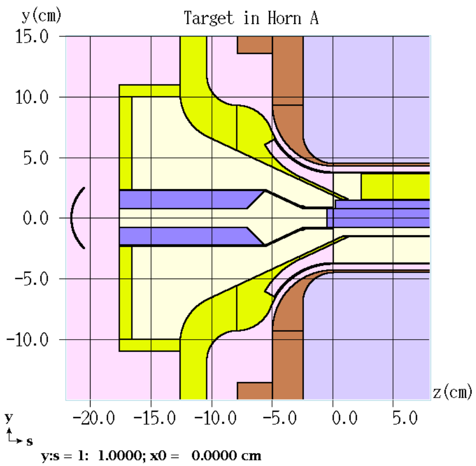
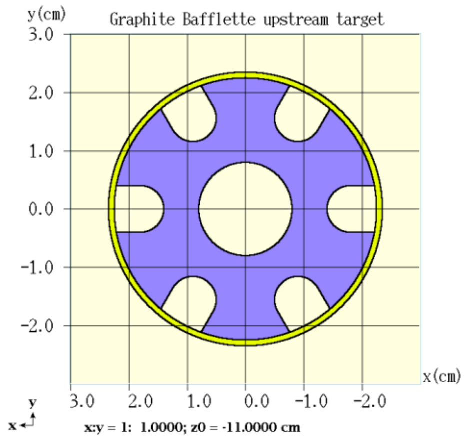
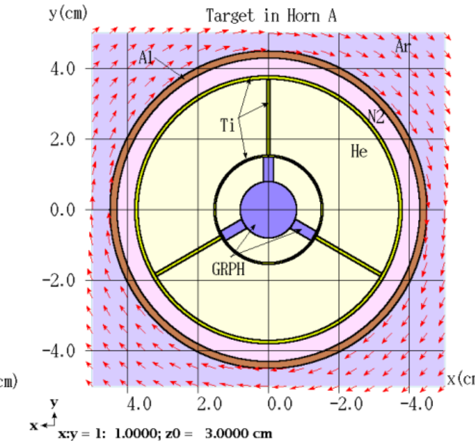
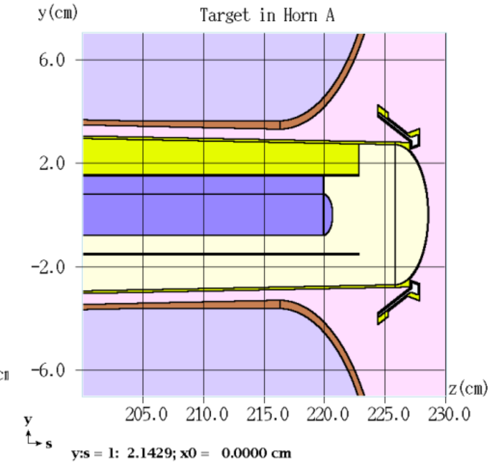
Details of the LBNF-MARS TS Model

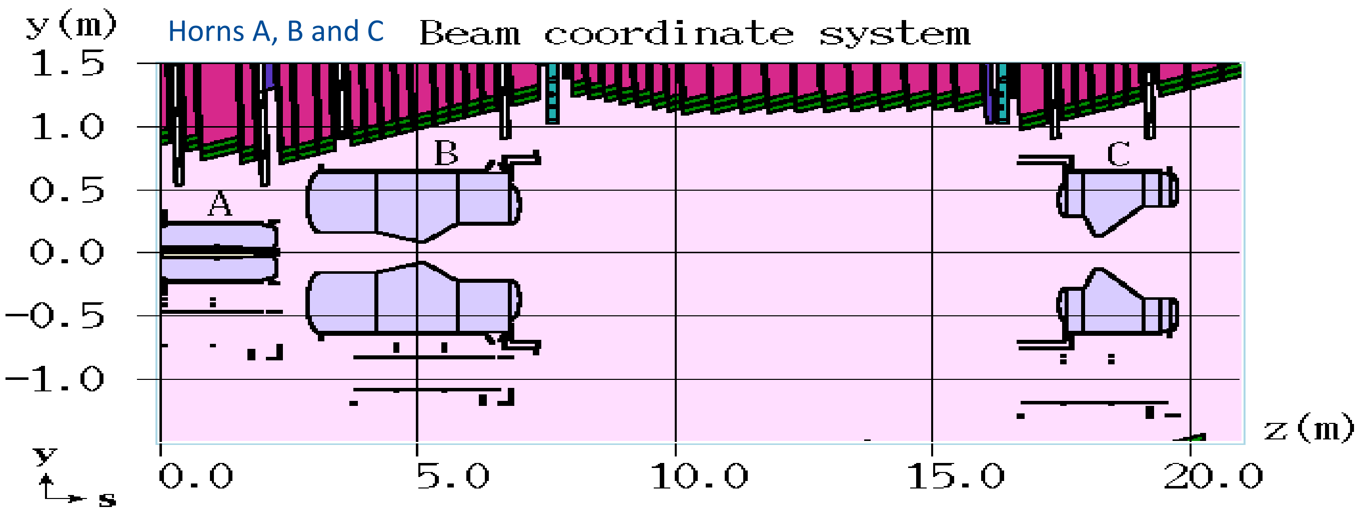




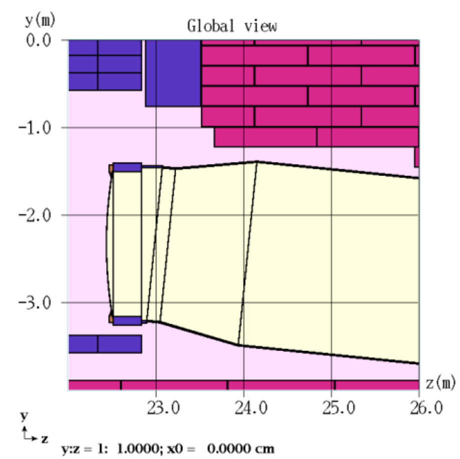




Horns A, B and C



Upstream of DK pipe

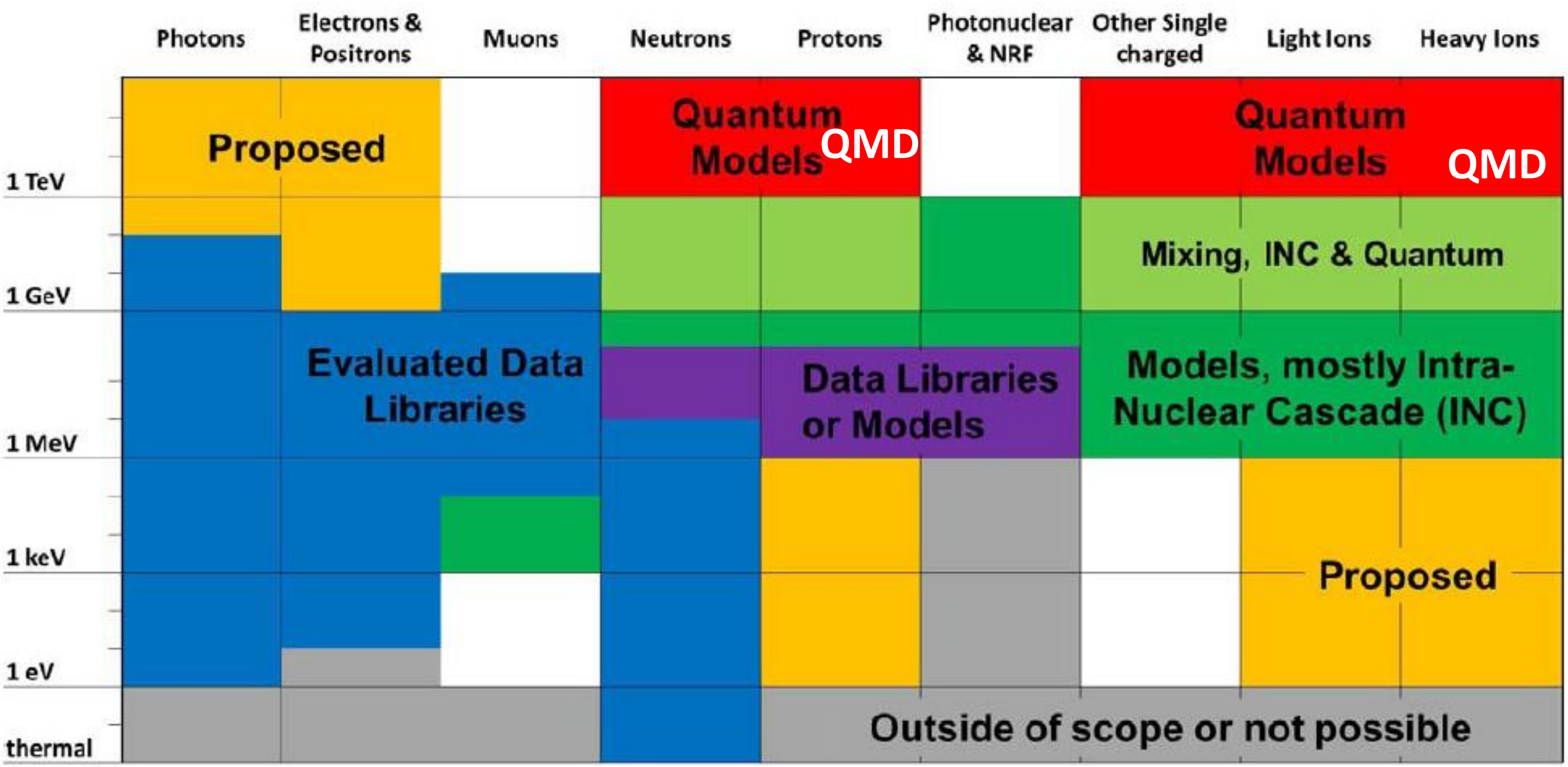


MCNP6 (mcnp.lanl.gov)

MCNP6 is the latest version of the Monte Carlo N-Particle transport (MCNP) family of particle interaction and transport codes (**Fortran-90**) and features comprehensive and detailed descriptions of the related physical processes. It transports 37 different particle types, including ions and electromagnetic particles. The neutron interaction and transport modules use standard evaluated data libraries mixed with physics models where such libraries are not available. ***Considered by many as the industry standard for simulation in reactor, medical, space and low- and medium-energy accelerator applications.***

The transport is continuous in energy. MCNP6 contains one of the most powerful implementations of variance reduction techniques. Spherical mesh weight windows can be created by a generator in order to focus the simulation time on certain spatial regions of interest. In addition, a more generalized phase space biasing is also possible through energy- and time-dependent weight windows. Other biasing options include pulse-height tallies with variance reduction and criticality source convergence acceleration.

MCNP6 Models



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MCNP6 Geometry, B-Field and Tests

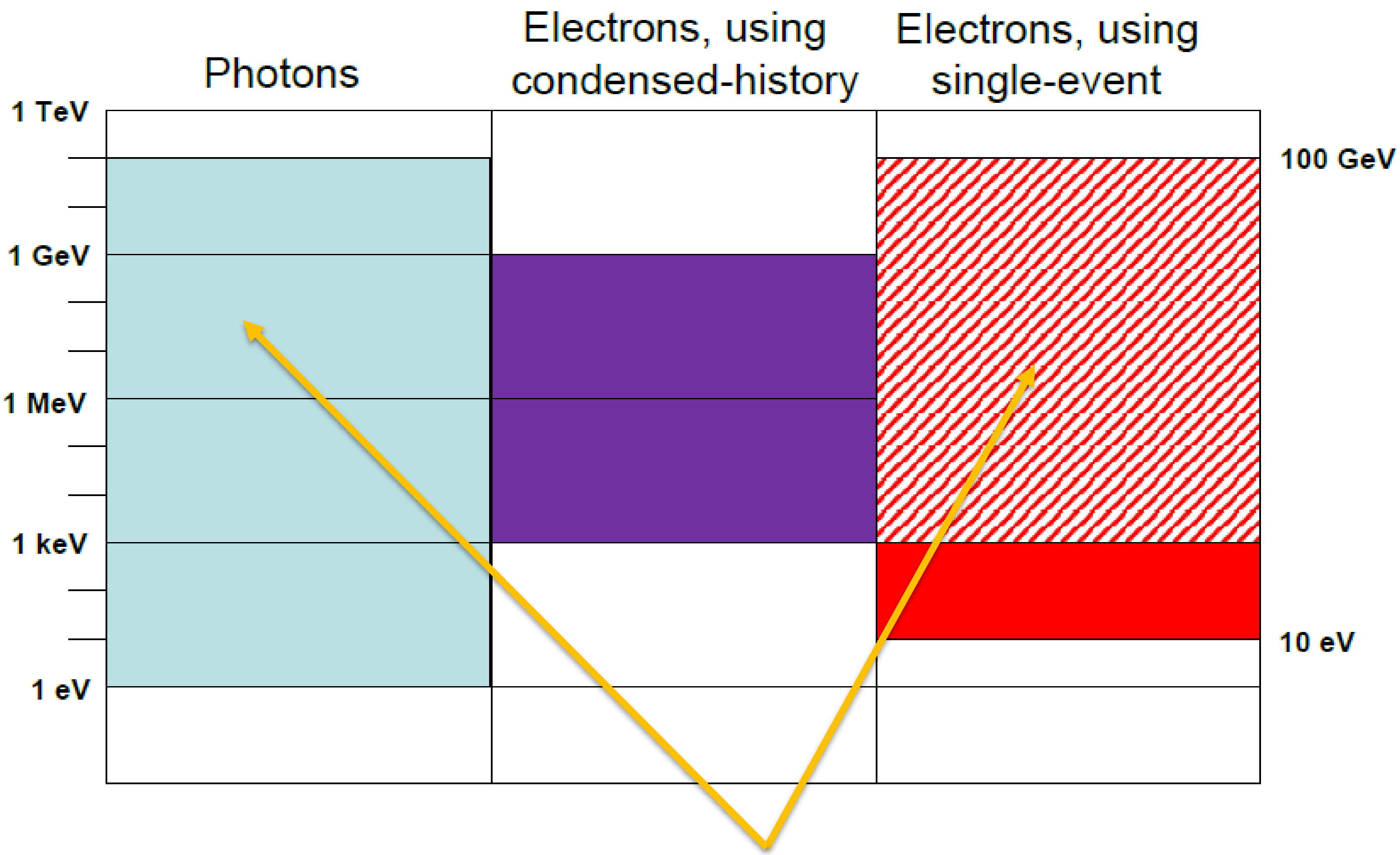
- Geometry options: traditional surface-based, voxel lattice, constructive solid and unstructured mesh

- Magnetic fields: (1) Constant dipole, square-edge quadrupole and quadrupole with a fringe-field kick – all in low-density materials, such as air; (2) COSY maps only in vacuum and specific to one particle type; both are rather limited compared to four other codes with the arbitrary EM field capability in arbitrary geometry/materials

- **Unique feature:** MCNP6 is considered risk level two software (death is risk level one), i.e. is treated as if failure of the software could result in temporary injury or illness to workers or the public. Therefore, a set of hundreds automated verification, validation and regression tests. Latter is detecting unintended changes to the code and installation testing.

- Super-precise simulation of EMS at 1 eV to 100 GeV

MCNP6: Super-Precise Simulation of EMS



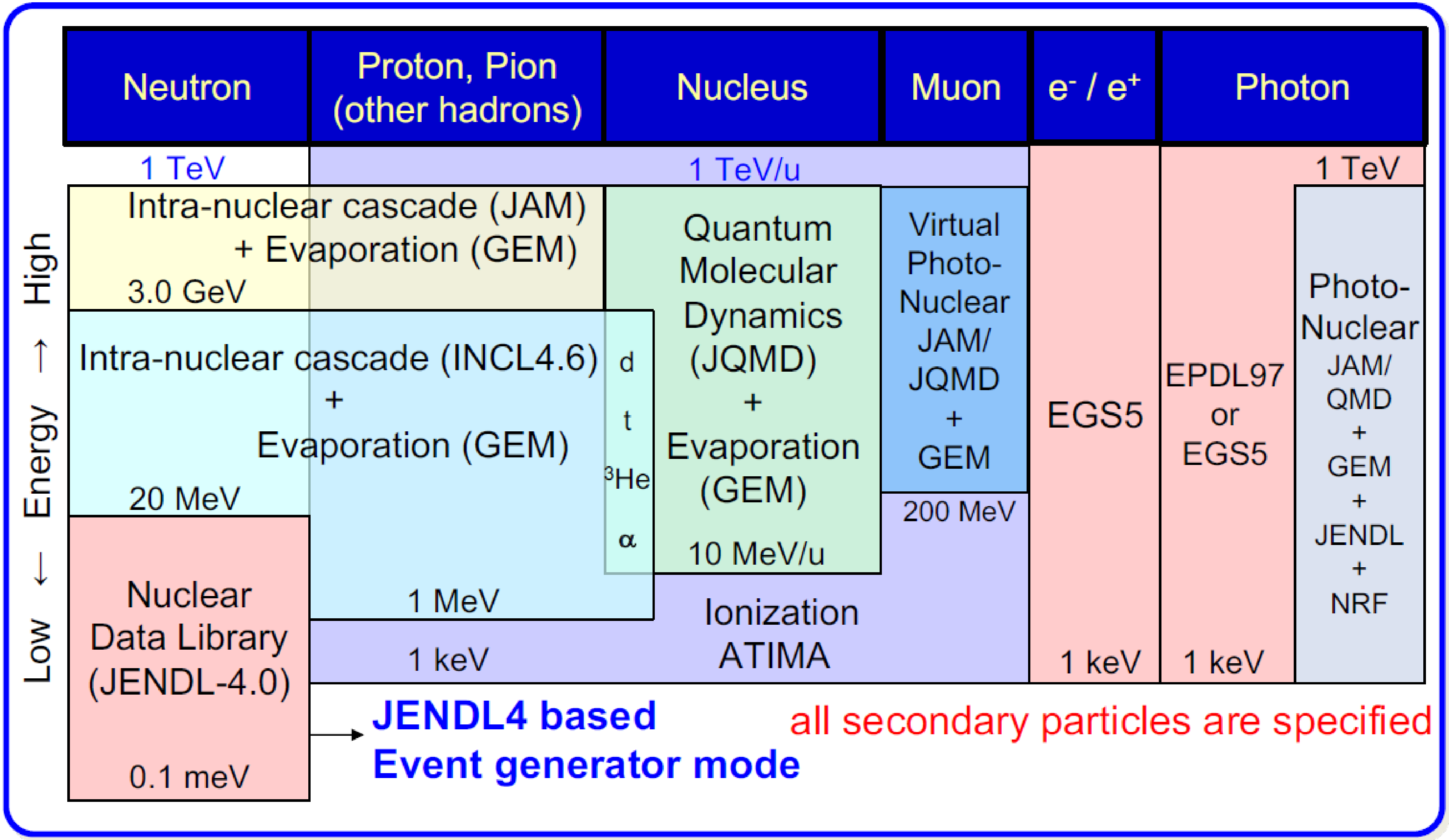
Can be very CPU-time consuming

PHITS (phits.jaea.go.jp)

PHITS is the Particle and Heavy-Ion Transport code System (**Fortran 77**). ***It was among the first general-purpose codes to simulate the transport and interactions of heavy ions in a wide energy range***, from 10 MeV/nucleon to 100 GeV/nucleon. It is based on the high-energy hadron transport code NMTC/JAM that was extended to heavy ions.

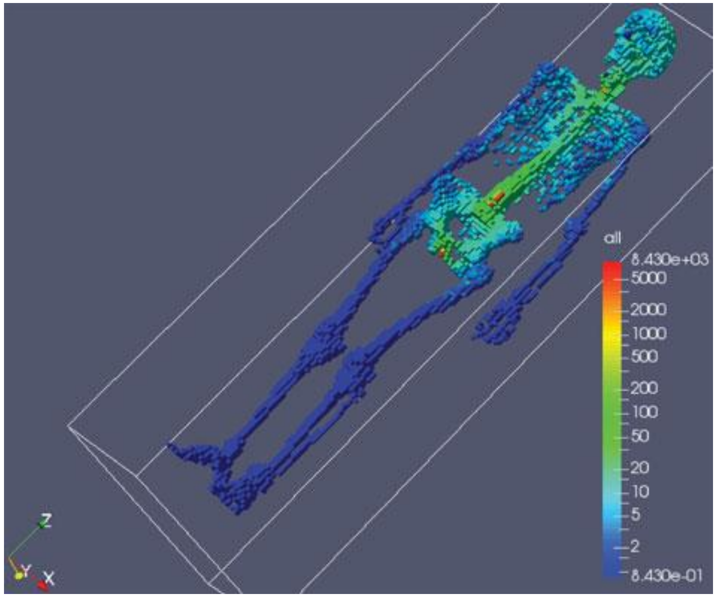
The transport of low-energy neutrons employs cross sections from evaluated nuclear data libraries such as ENDF and JENDL below 20 MeV. Electromagnetic interactions are simulated based on the EGS5 code in the energy range between 1 keV and 100 MeV for electrons and positrons and between 1 keV and 100 GeV for photons. Several variance reduction techniques, including weight windows and region importance biasing, are available. An accurate calculation of DPA supported by dedicated experiments with medium-energy protons.

PHITS Models



PHITS Geometry, Fields, Nuclides & Tallying

- The geometrical configuration of a simulation is set with general geometry (GG) in a manner similar to MCNP. The interactive solid modeler Simple-Geo (FLUKA) can be used for generating the geometries written in PHITS-readable GG format.
- Computer-aided Design (CAD)-based geometries can be incorporated into PHITS by converting CAD data into tetrahedral-mesh geometries. In addition, CAD geometries can be directly converted into the PHITS-readable GG format by using SuperMC.



- Electromagnetic fields and gravity can be considered in transport simulation of all particles.
- The time evolution of radioactivity is estimated by built-in DCHAIN-SP module.
- An example of tallying is shown

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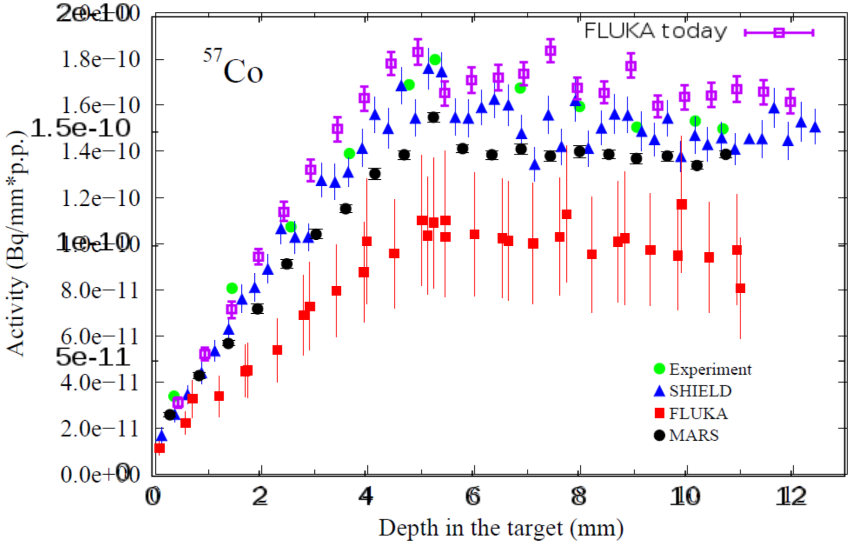
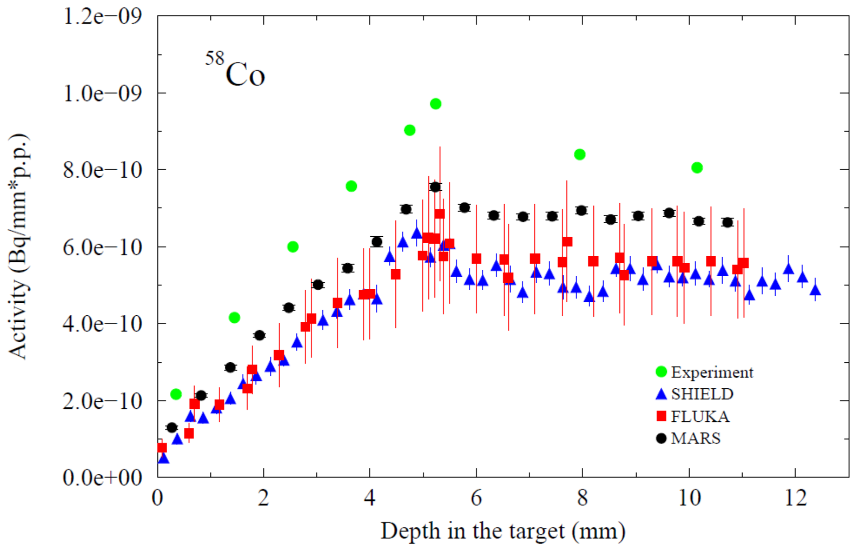
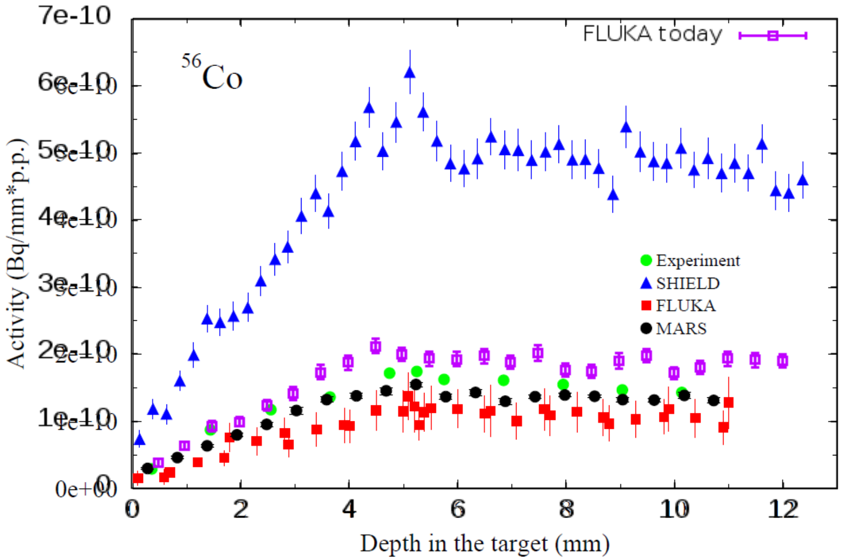
Activity Benchmarking at GSI

500 MeV/n ^{238}U beam on Cu

[E. Mustafin *et al.*, EPAC 2006, TUPLS141, 1834]







CERN CHARM Facility at 24 GeV/c

T. Oyama et al.

Nuclear Inst, and Methods in Physics Research B 434 (2018) 29–36

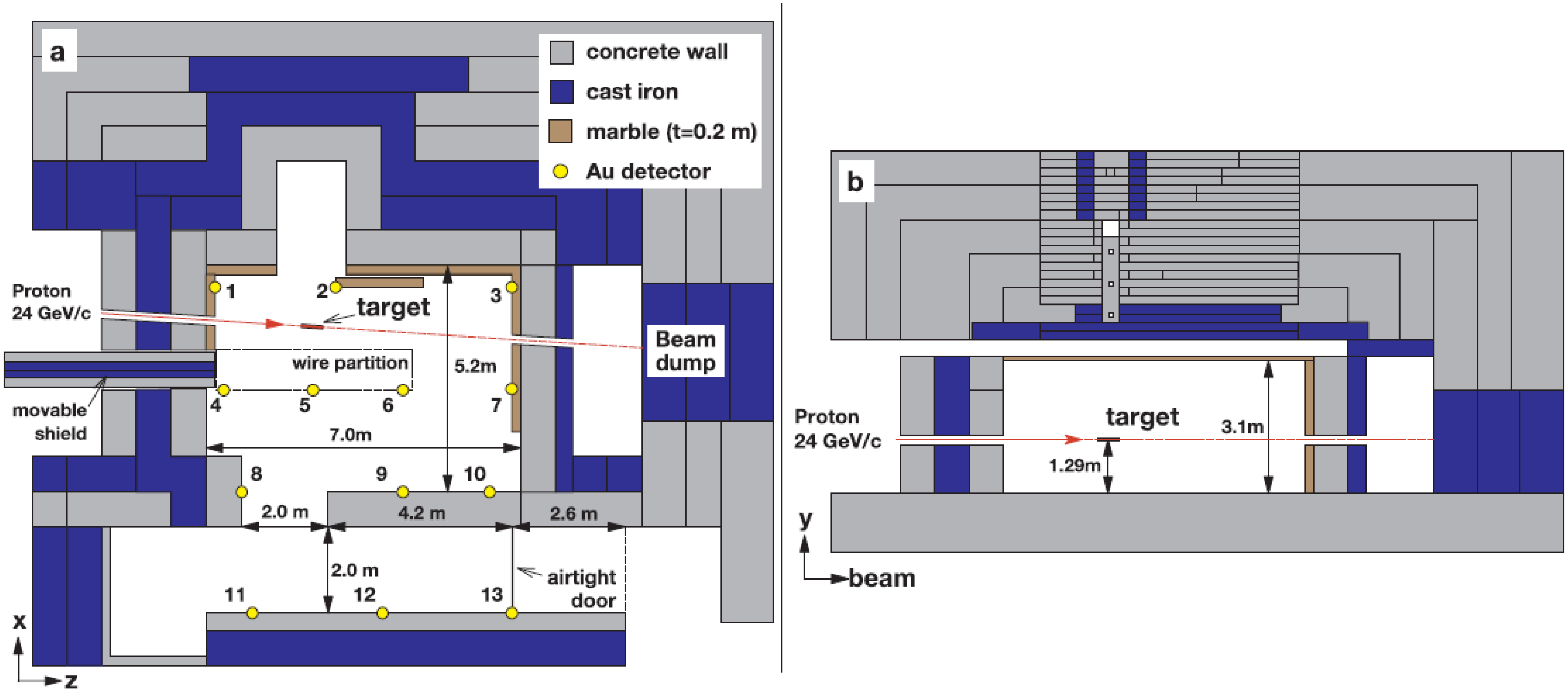
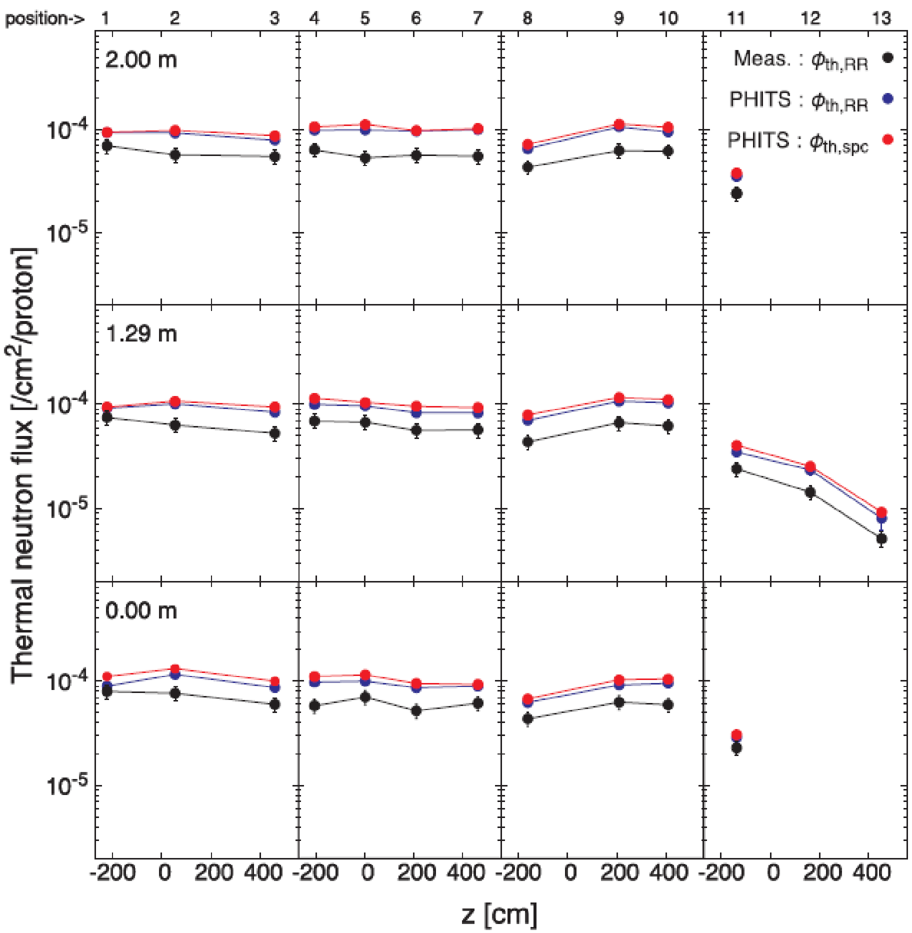
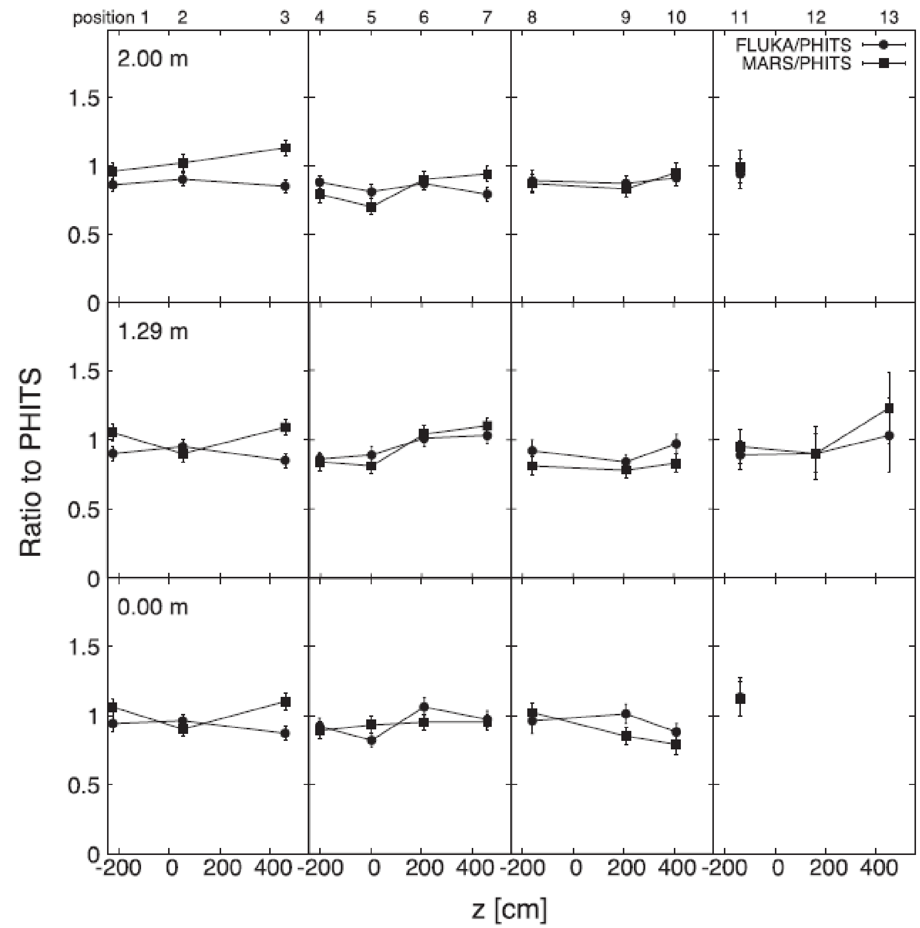


Fig. 1. Cross-sectional view (a) and longitudinal-sectional view (b) taken along the Cu target plane of the CHARM facility, together with important dimensions. The numbers 1–13 indicate the experimental location of the gold foils.

PHITS, FLUKA & MARS *vs* CHARM 24 GeV/c Data



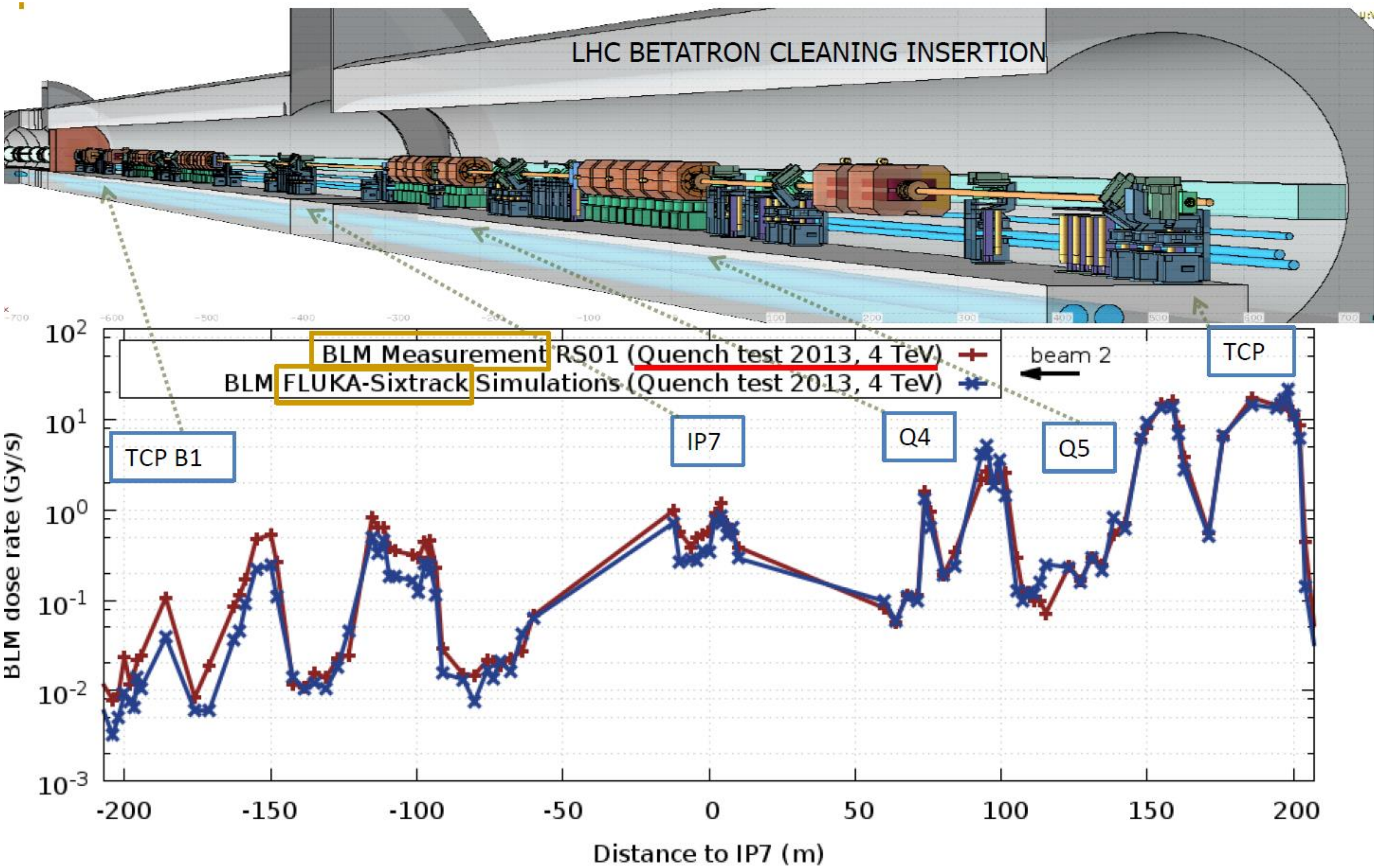
PHITS & Exp within 50%



FLUKA, PHITS & MARS within 30%

T. Oyama et al., NIM, **B434** (2018) 29-36

FLUKA Verification at LHC Betatron Cleaning

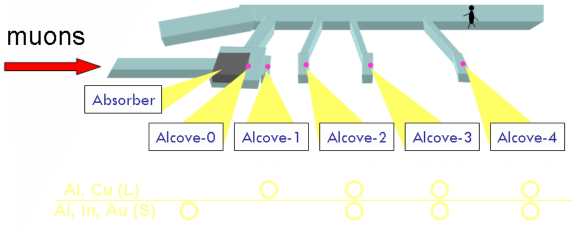


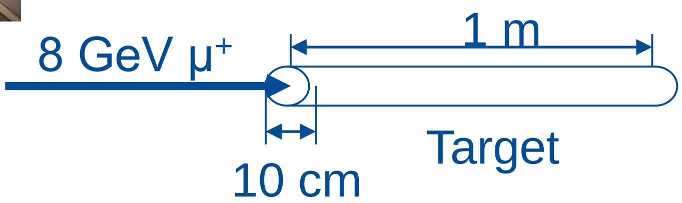
Fermilab

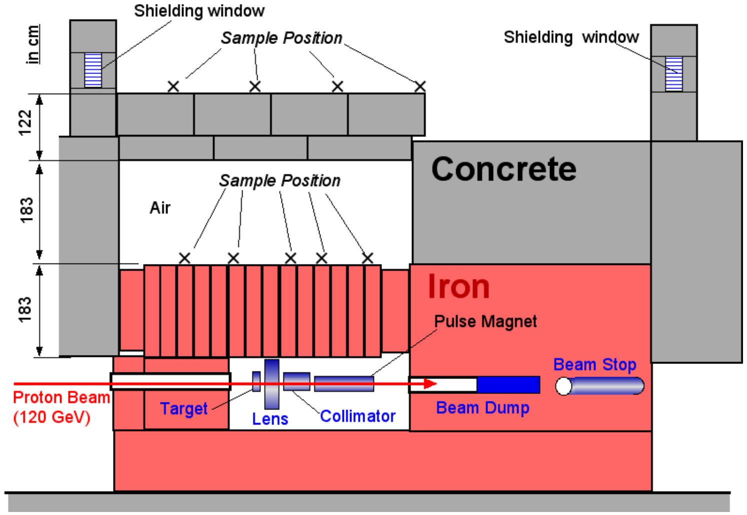
Shielding and Radiation Effect Experiment

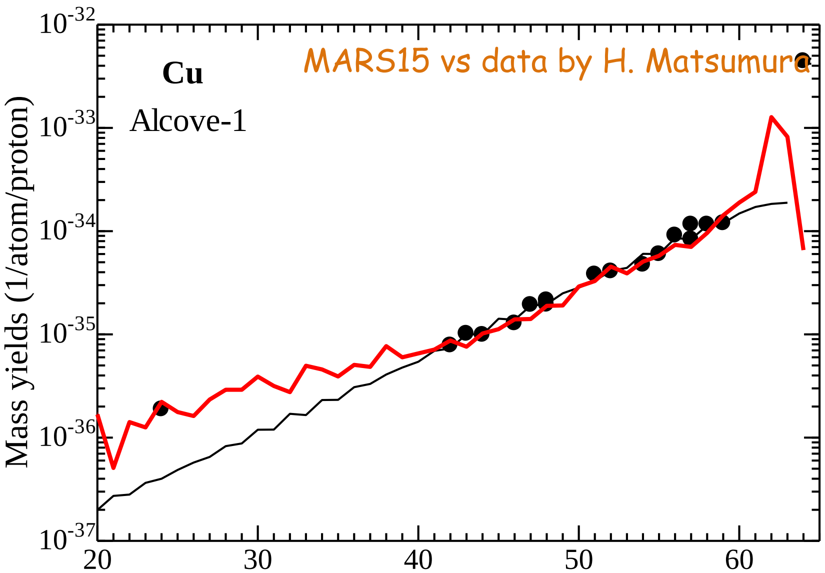
JASMIN Japan-FNAL Collaboration:
<u>Shielding and Radiation Effect Experiments at FNAL</u>
T-972 (2007-2009)
T-993 and T-994 (2009-2012)
Shielding data and code benchmarking; targets, collimators and thick shields; radiation effects on instruments and materials

Example: Muon-induced nuclide production









Air Activation at NuMI Neutrino Production Facility

To get more confidence in the MARS15-based LBNF target station design, a benchmarking campaign on air activation has been recently undertaken at the Fermilab NuMI target station for 120-GeV beam on target

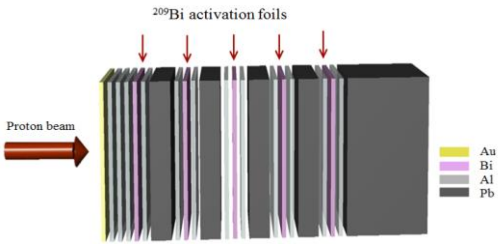
NIM **B414** (2018) 4-10

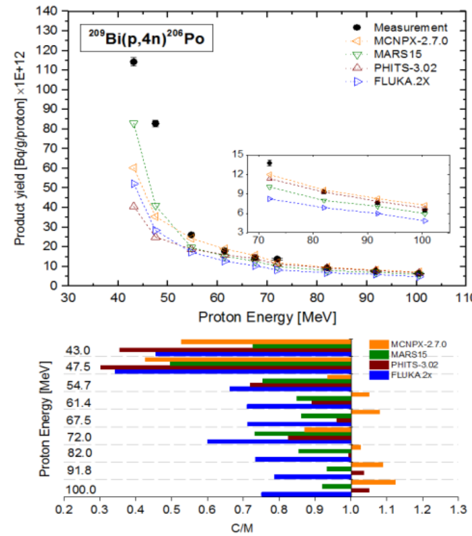
Measured and calculated production rate density (cm^{-3} POT^{-1} s^{-1}) for the most important radionuclides generated in the air in the beam enclosure of the NuMI target chase.

Production rate	^{41}Ar	^{11}C	^{13}N	^{15}O
Measurement	1.98×10^{-12}	6.38×10^{-11}	4.07×10^{-11}	3.50×10^{-11}
Standard methodology	6.85×10^{-12}	2.22×10^{-10}	5.22×10^{-11}	9.16×10^{-11}
MARS15	1.08×10^{-12}	4.44×10^{-11}	3.71×10^{-11}	4.16×10^{-11}
MARS15/data	0.55	0.70	0.91	1.19

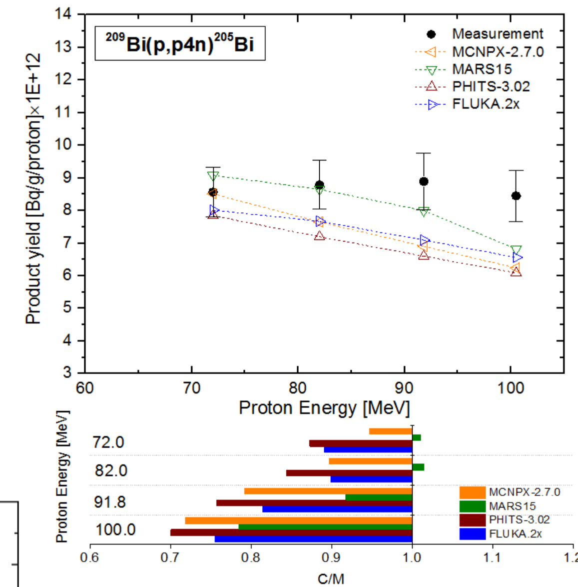
50% 10-30%

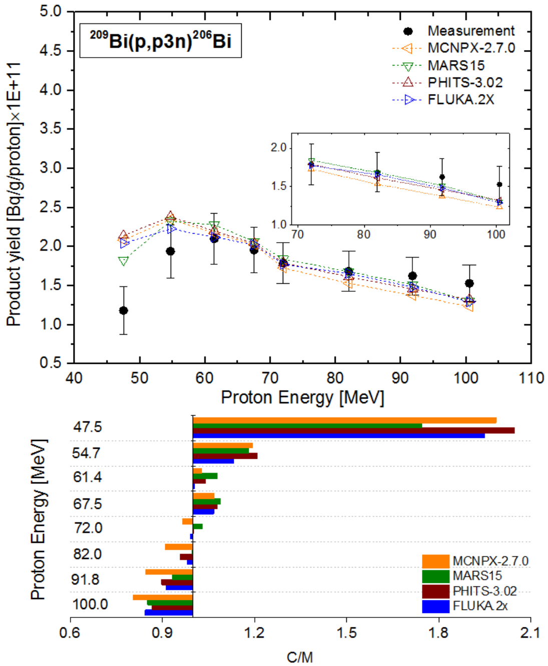
FLUKA, PHITS, MCNPX and MARS15 Benchmarking

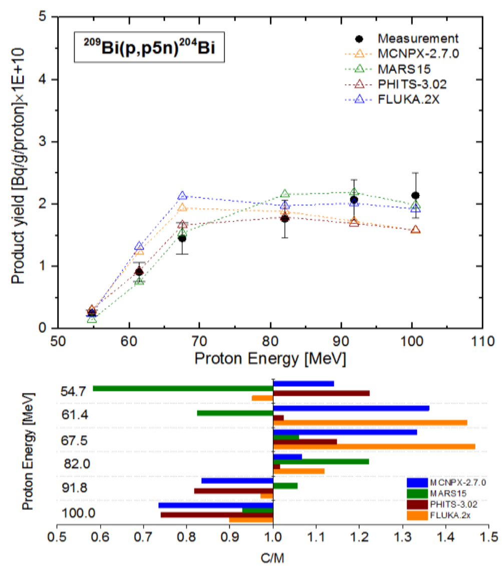




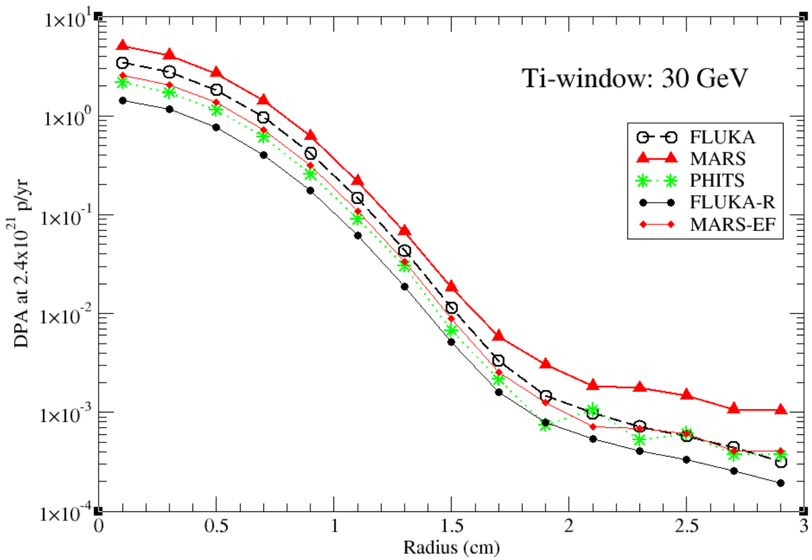
L. Mokhtari et al., NIMB 462 (2020) 154-162

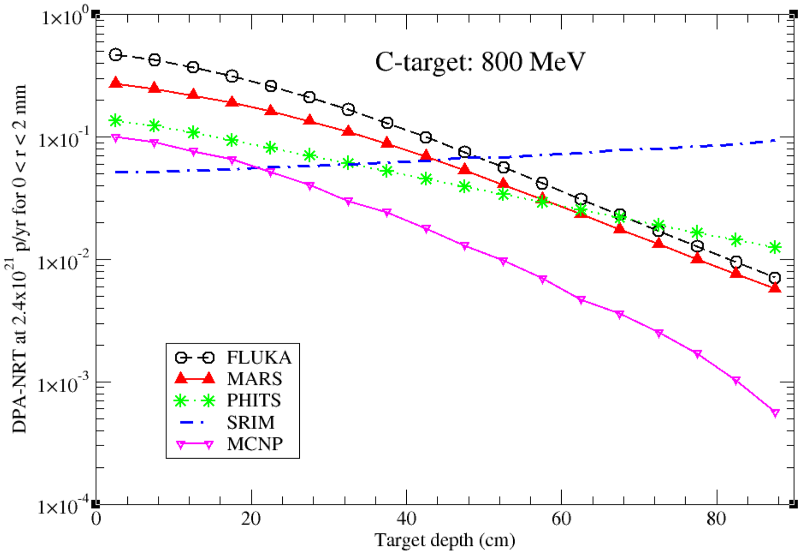


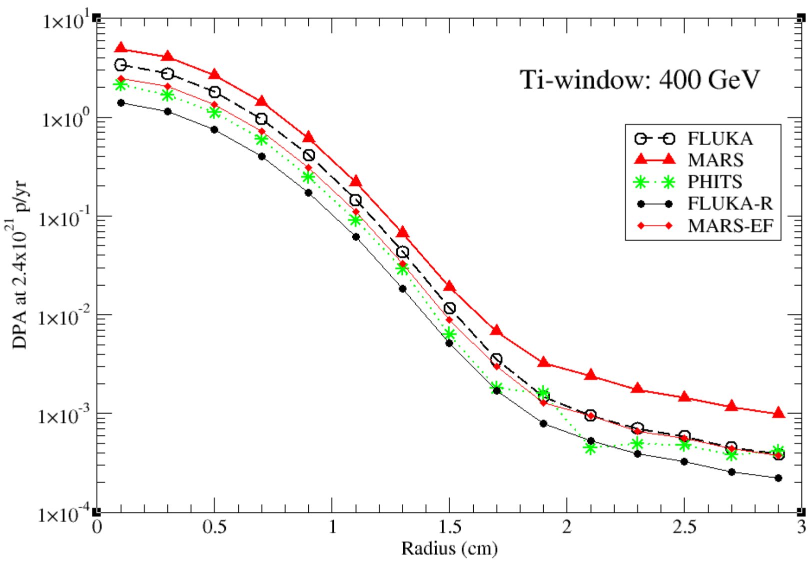


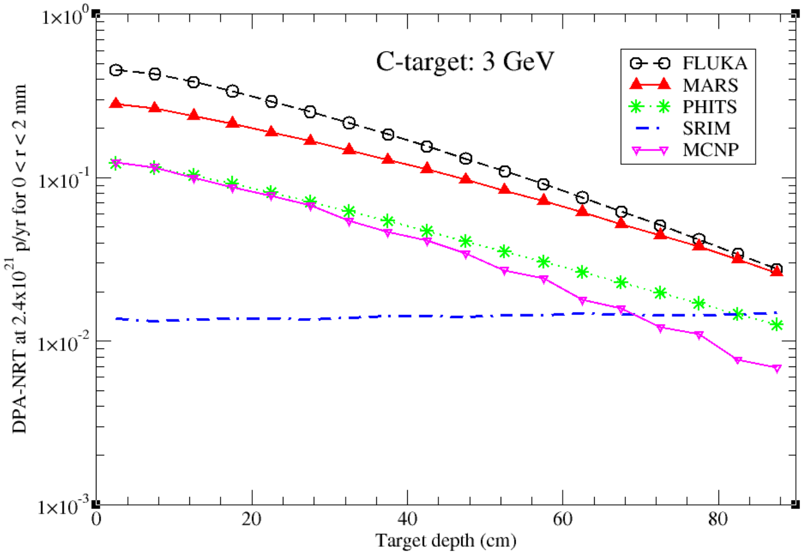


DPA Code Intercomparison in Ti-Window and C-Target









Input Files

The user creates input files that are subsequently read by the code. These files contain info about the problem in areas such as:

1. Geometry specification with material assignment to the regions
2. Description of materials
3. Scoring/tallying definition - “sensitive region” assignment in item (1) or/and geometry-independent mesh/histograms with corresponding lists of functionals
4. Possible assignment of magnetic and electric fields and other properties affecting particle transport in regions of item (1)
5. The source term either in a simple parametric form or as an external file
6. The cutoff energies or/and time of flight (TOF) for particle classes, materials and regions
7. Possible material/region spatial resolution and pilot steps
8. Any variance reduction techniques to be applied for various interaction classes, regions, materials etc.

Rules-of-Thumb for MC Code Users

1. Define and sample the geometry and source well
2. You cannot recover lost information
3. Question the stability and reliability of results
4. Be conservative and cautious with variance reduction biasing
5. The number of histories run is not indicative of the quality of the results; rather aim at a RMS statistical error less than a few % in the regions of interest
6. In short runs, try to understand what a combination of variance reduction techniques provides the highest computing efficiency and estimate required total number of histories
7. Use biasing in particle-, cutoff energy-, space- and material--dependent manner
8. Minimize the number of unneeded regions and histograms