Particle – Matter Interaction Simulations in Accelerator Applications

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Outline

- Introduction
- Interactions of Fast Particles with Matter
- Materials Under Irradiation: An Example of Particle-Matter Interaction and its Importance in Accelerator Applications
- Modern State-of-the-Art Monte-Carlo Codes
- Code Structure, Features, and Applications
- Code Benchmarking: Validation, Intercomparison, Verification
- Summary

Based on the materials of the lectures “Simulation of Particle – Material Interactions”, taught by the MARS particle-matter code creator and the MARS group leader at Fermilab, Nikolai Mokhov, at CERN Accelerator School in Thessaloniki, Greece, on 11-23 November 2018

Introduction

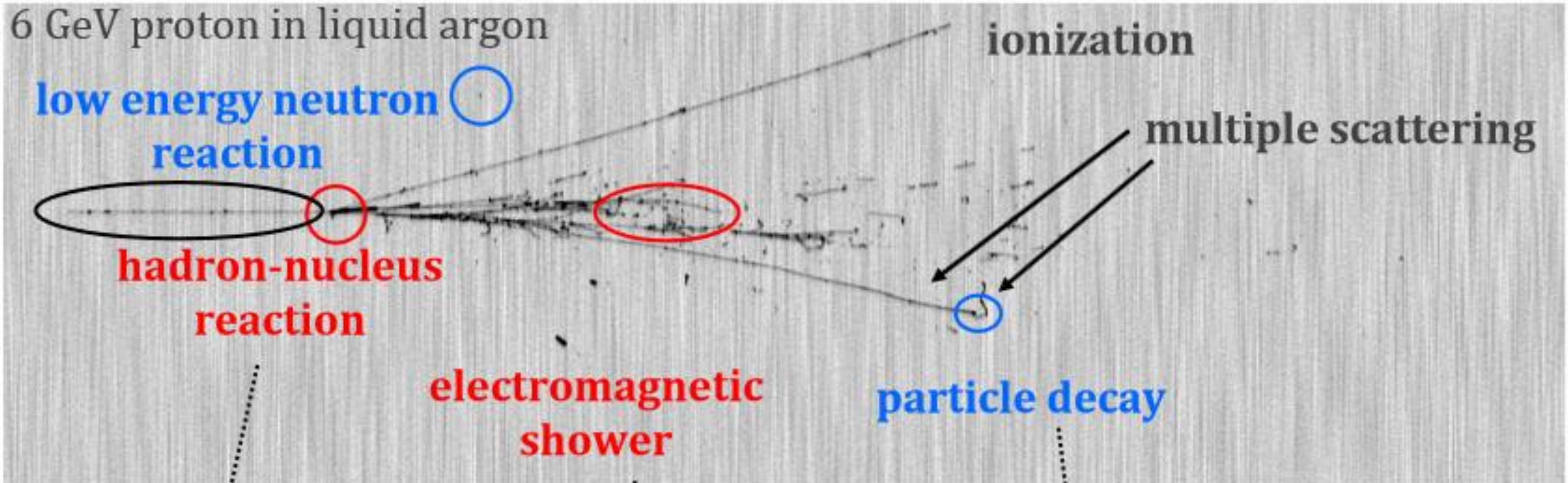
- The consequences of controlled and uncontrolled impacts of various particle beams on accelerator beamline components can range from minor to catastrophic.
  - High-intensity and/or high-power and/or high-energy beams
  - Target stations, beam collimators, absorbers, detectors, shielding, environment can be affected
- Strong, weak, electromagnetic and even gravitational forces govern high-energy beam interactions with complex components.
  - Simulations are only possible with a few well-established Monte-Carlo codes
  - Analytical or simplified approaches are used only for code verification
- Predictive power and reliability of particle transport simulation tools and physics models in the multi-TeV region should be well-understood and justified to allow for viable designs of future colliders with a minimal risk and a reasonable safety margin.

Interactions of Fast Particles with Matter

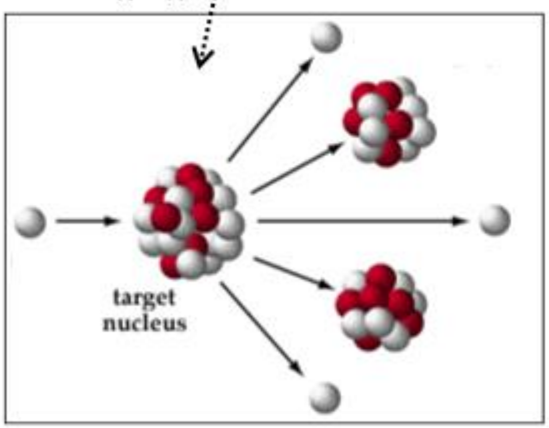
Electromagnetic interactions, decays of unstable particles and strong inelastic and elastic nuclear interactions all affect the passage of high-energy particles through matter. At high energies the characteristic feature of the phenomenon is creation of hadronic cascades and electromagnetic showers (EMS) in matter due to multi-particle production in electromagnetic and strong nuclear interactions.

Because of consecutive multiplication, the interaction avalanche rapidly accrues, passes the maximum and then dies as a result of energy dissipation between the cascade particles and due to ionization energy loss. Energetic particles are concentrated around the projectile axis forming the shower core. Neutral particles (mainly neutrons) and photons dominate with a cascade development when energy drops below a few hundred MeV.

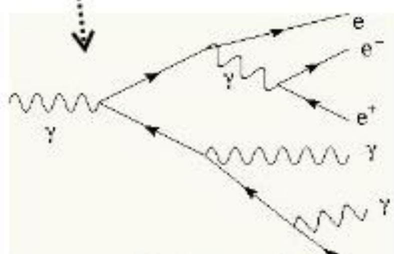
Microscopic View



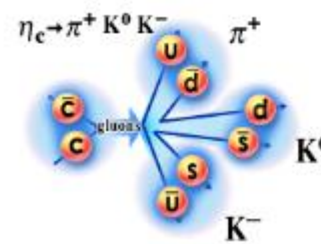
$$\lambda\rho = \frac{A}{\sigma_R N_A} \qquad \sigma_R \simeq \pi r_0^2 A^{2/3}$$



interplay of many physical processes described by different theories/models



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



Fermilab

Materials Under 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 direct particle beams or secondary radiation induced by these beams.

Component damage (lifetime):

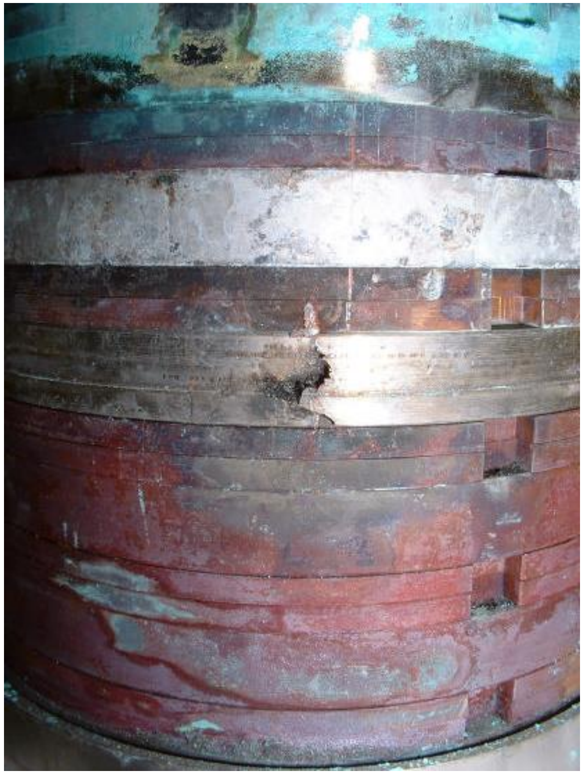
- Thermal shocks and quasi-instantaneous damage
- Insulation property deterioration due to dose buildup
- Radiation damage to inorganic materials due to atomic displacements and helium production

Operational (performance):

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

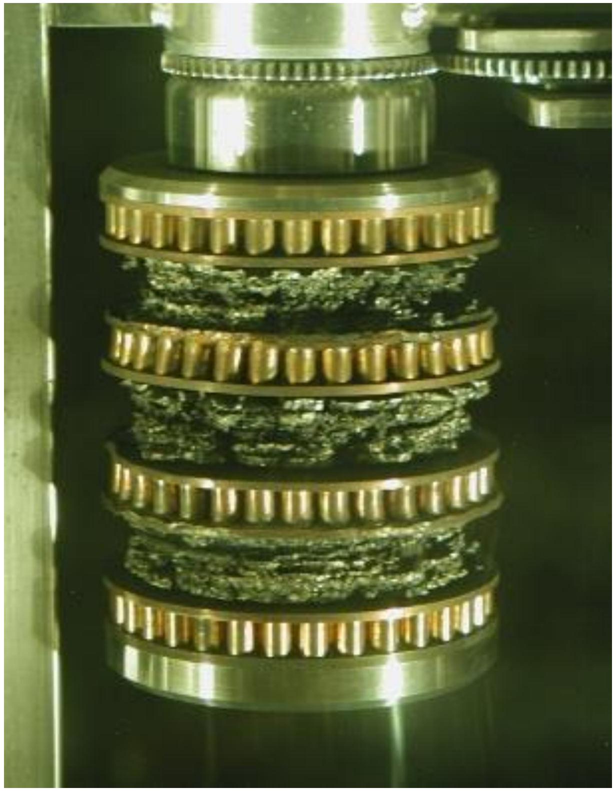
Example: Thermal Shock

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



FNAL pbar production target under 120-GeV p-beam (3e12 ppp, $\sigma \sim 0.2$ mm)

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



Particle Transport in Matter: Monte-Carlo Method

- The **Monte-Carlo (random walk) method** is the major technique used in particle transport applications. It involves numerical simulations of the interactions and propagation of particles in matter (***direct mathematical modeling***). All the physics processes are modelled as realistically as possible, using realistic geometry and materials, as well as accelerator fields (electromagnetic) and experimental setup.
  - The use of various modifications, the so-called ***variance reduction techniques***, helps simplify the solution in certain cases, yet retaining high accuracy of the result.
- Codes can calculate directly: spatial distribution of energy deposition density, heat loads (e.g., to evaluate absorbed dose), particle fluence, star density, prompt and residual effective dose, isotope production, air and water activation, and various other quantities.

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, associated extensive benchmarking with experimental data and related code developments, **the modeling has reached an unprecedented accuracy**.

FLUKA, GEANT4, MARS15, MCNP6 and PHITS

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 multi-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.

FLUKA (www.fluka.org)

FLUKA is a general-purpose particle interaction and transport code. It contains all features needed for radiation protection calculations, 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. 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.**

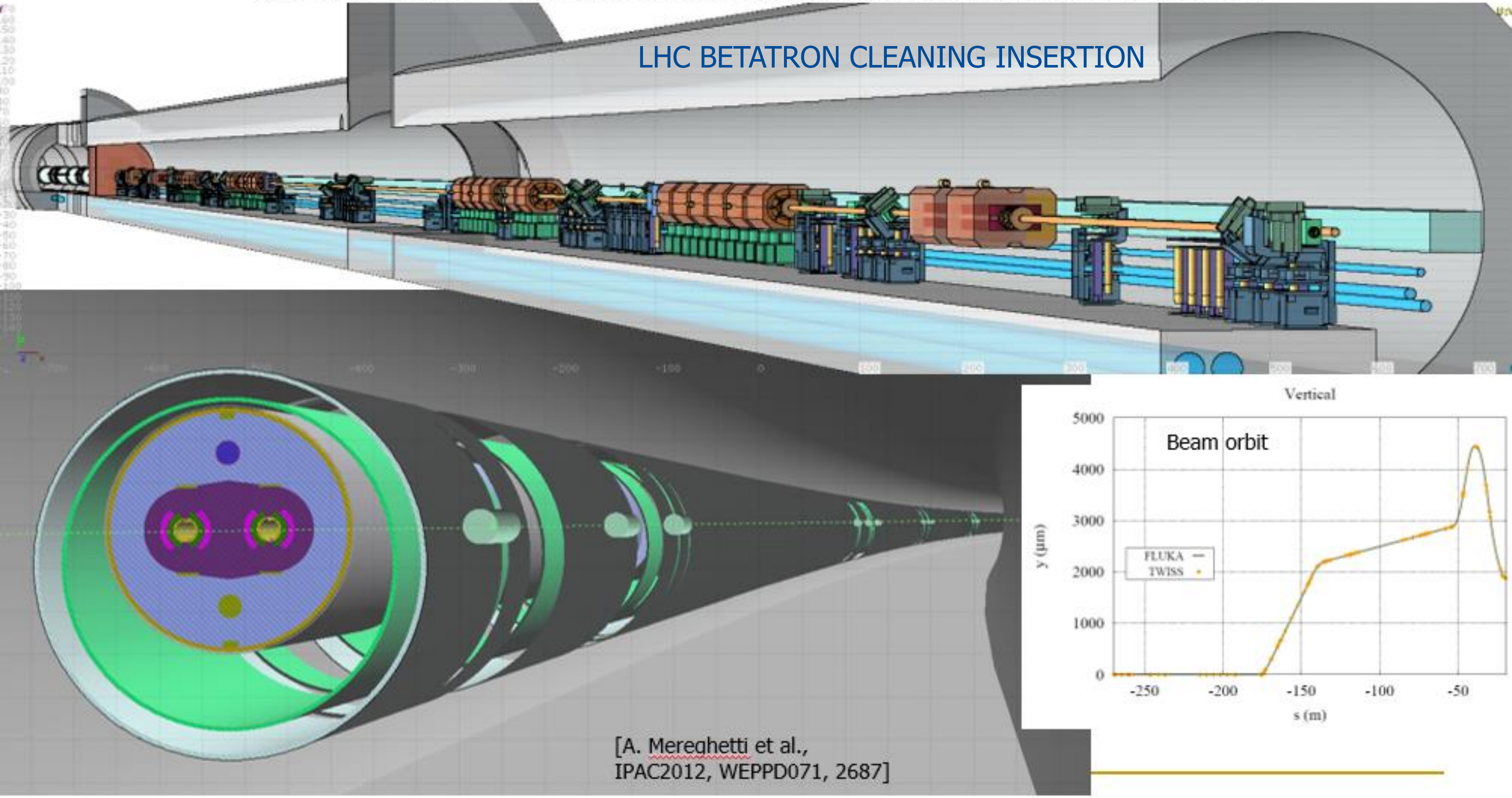
FLUKA Features

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 visualization 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 in a fully analogue mode. 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

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



[A. Mereghetti et al.,
IPAC2012, WEPPD071, 2687]

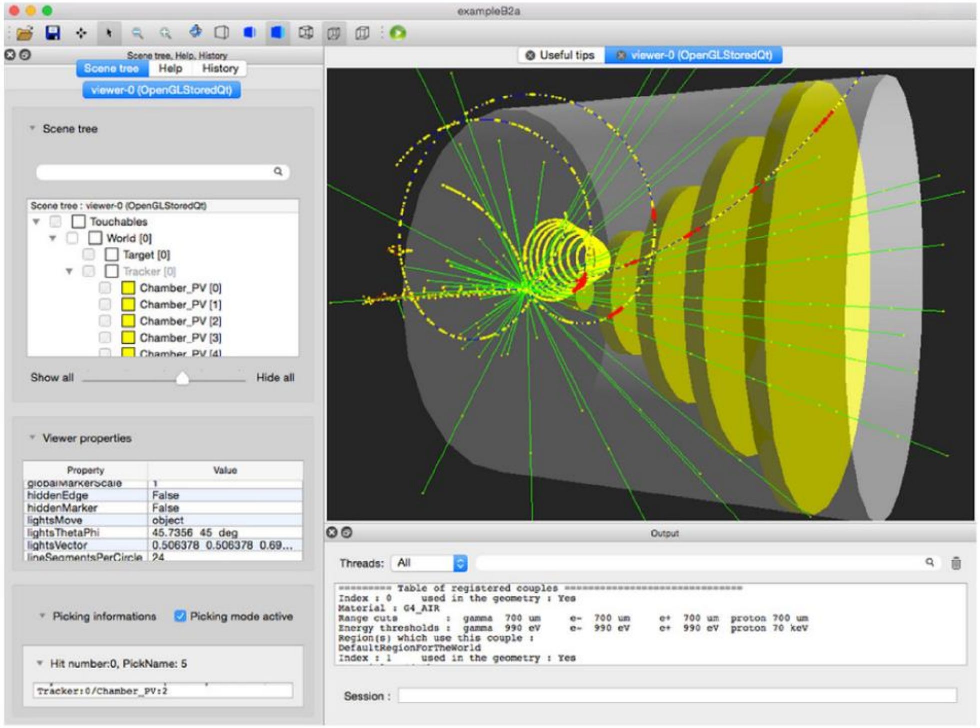
C++

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.

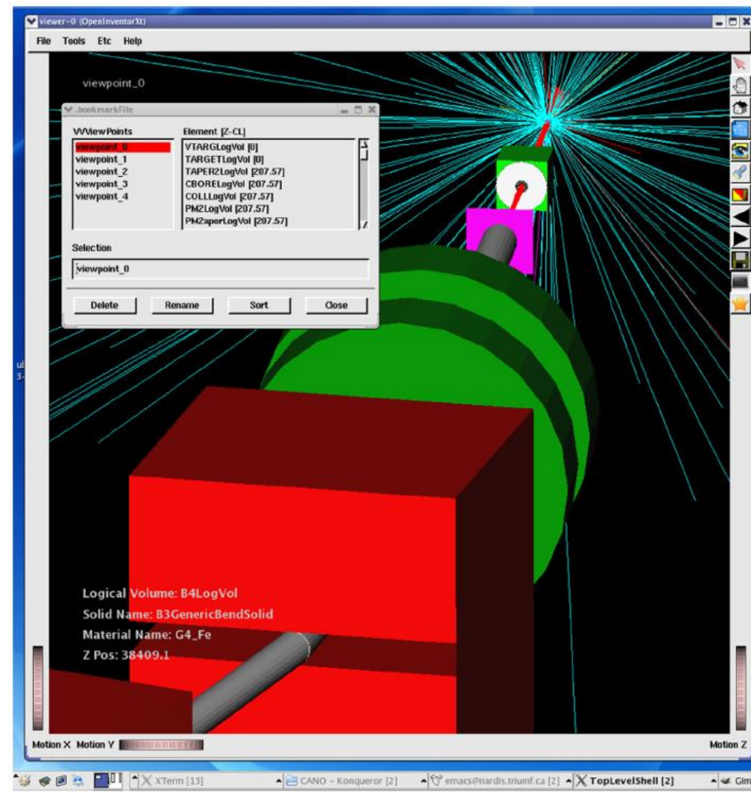
G4 is the industry standard for HEP detector simulation. To facilitate the use of variance reduction techniques, general-purpose biasing methods such as importance biasing, weight windows, and a weight cut-off method have been introduced directly into the toolkit. Other variance reduction methods, such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

GEANT4: Viewers



OpenGL viewer wrapped in Qt

Open inventor extended viewer



Fortran-77 & C++

MARS15 (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

These applications are common for all 5 codes

MARS15 Features

- MARS15 is a set of programs for Monte-Carlo simulations of coupled hadronic and electromagnetic cascades, with heavy ion, muon and neutrino production and interaction. It covers a wide energy range: 1 keV to 100 TeV for muons, hadrons, heavy ions and electromagnetic showers; and 10^{-5} eV to 100 TeV for neutrons.
- Nuclear interactions as well as practically all other strong, weak and electromagnetic interactions in the entire energy range can be simulated either inclusively or exclusively – i.e, in a biased mode or in a fully or partially analogue mode.
- 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 handle interactions of neutrons with energies below 14 MeV and derive the NRT/Stoller/Nordlund DPA x-sections below 200 MeV. The elemental distributions are automatically unpacked into isotope distributions for both user-defined and those from the 172 built-in materials.

MARS15: Other Features

- 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.

- Six ways to describe geometry are offered, with a basic solid body representation and a ROOT-based powerful engine among them.

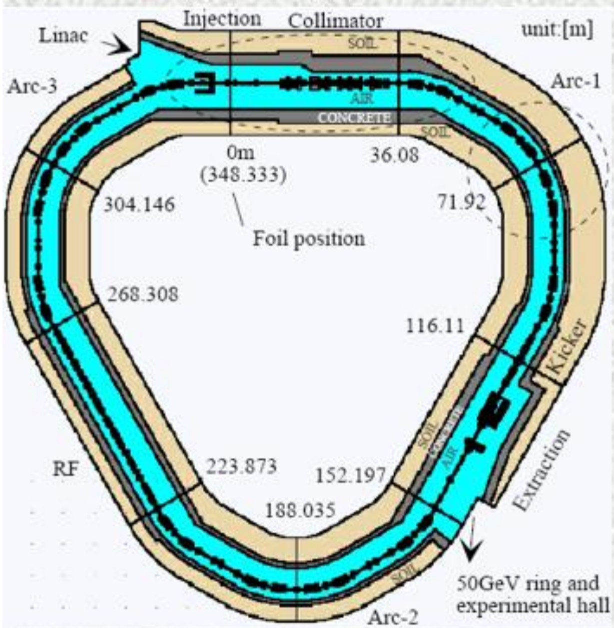
- ***The powerful capabilities of MARS15 for simulation in accelerator environment*** are the MARS-MAD Beamline Builder (**MMBLB**) working in concert with an accelerator tracking code (since almost 20 years ago) and a recent active merge with MADX-PTC for a convenient creation of accelerator models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

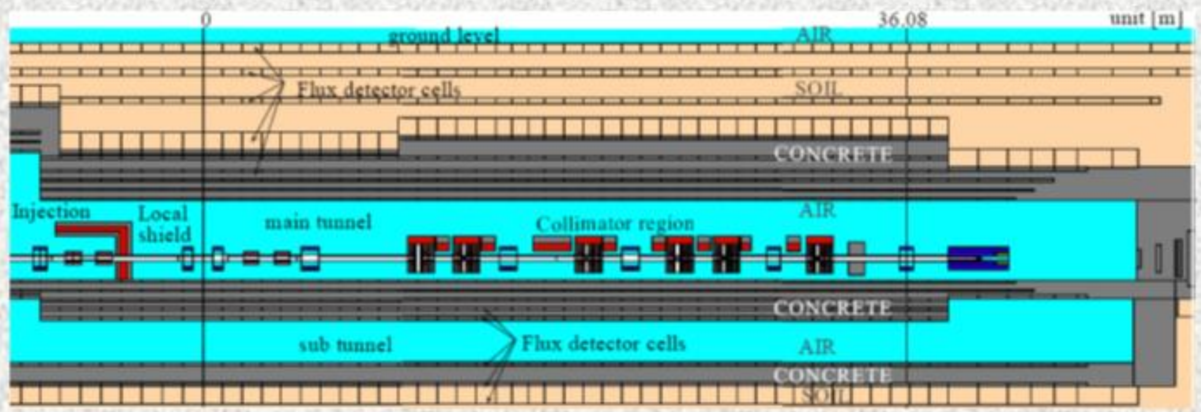
- MARS15 is routinely used in concert with ANSYS for iterative studies of thermo-mechanical problems and can be interfaced to a hydrodynamic code to study phase transition and "**hydrodynamic tunneling**" – first done at SSC for a 20-TeV proton beam in 1993.

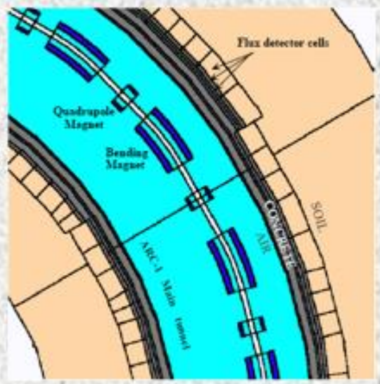
Geometry Description and ROOT-based Beamline Builder

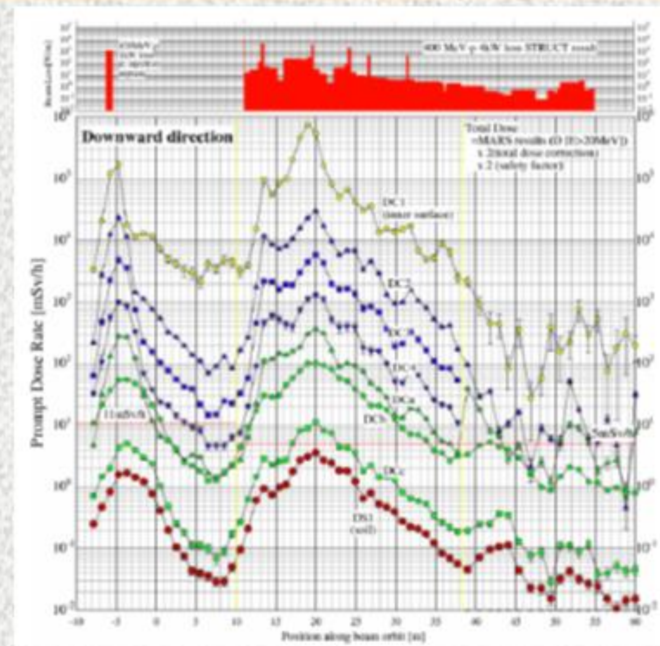
1. User-generated via MARS extended geometry input files
2. User-generated ROOT files
3. GDML files (two-way exchange with Geant4 teams)
4. G4beamline's BruitDeFond can generate MARS's input files MARS.INP, GEOM.INP and FIELD.INP
5. STEP files from project CAD models used to generate ROOT geometry modules
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

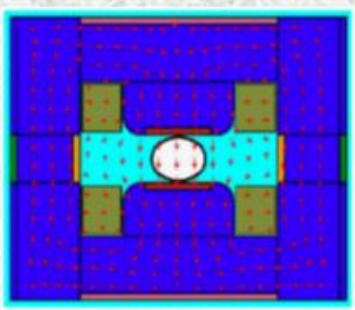
MMBLB Model: J-PARC 3-GeV Ring

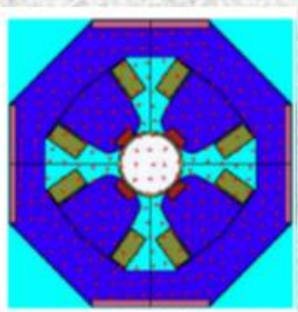




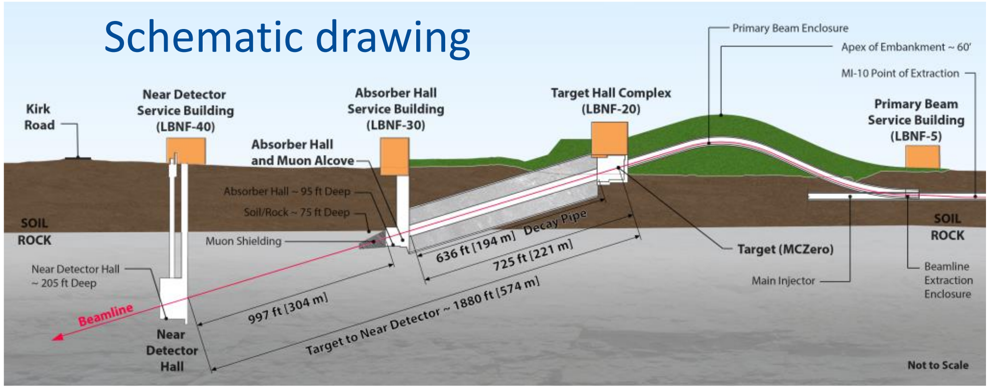


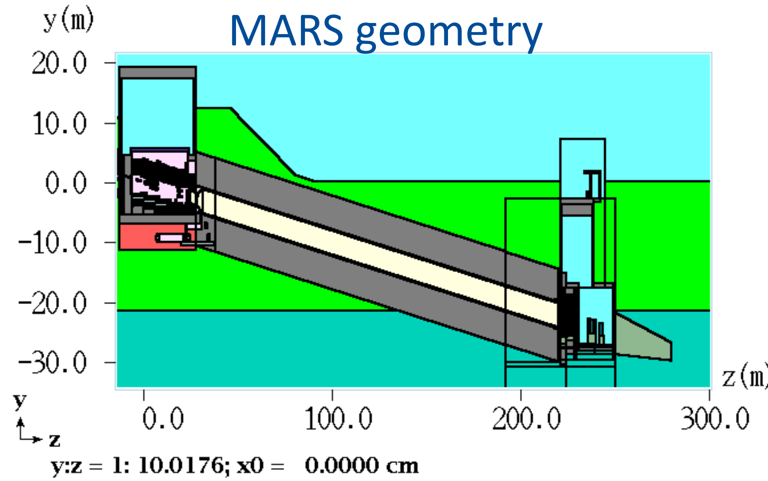






LBNF Beamline: MARS Model

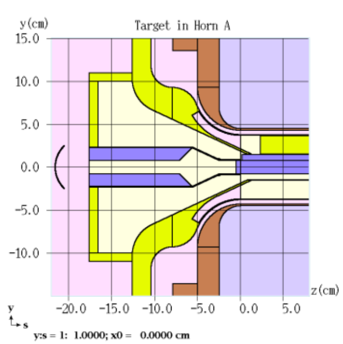


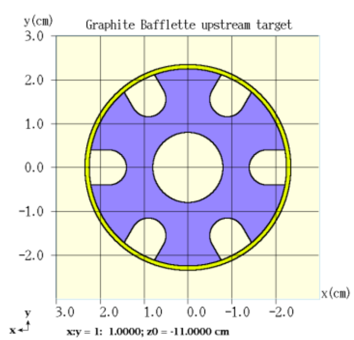


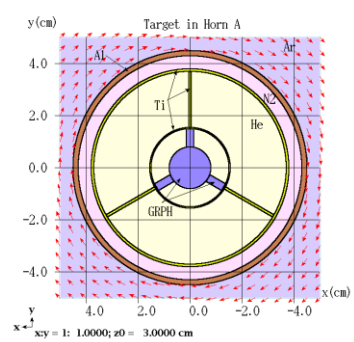
LBNF and DUNE

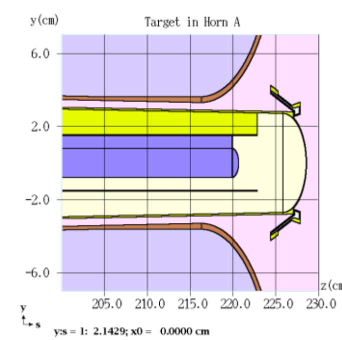
- Neutrinos from 60 to 120 GeV proton beam
- **1.2 MW from day one**; upgradeable to 2.4 MW
- **Near detector** to characterize the beam
- Massive underground LAr TP Chambers
- **4 x 17 kton** (fiducial mass of more than 40 kton)

Details of the LBNF MARS model



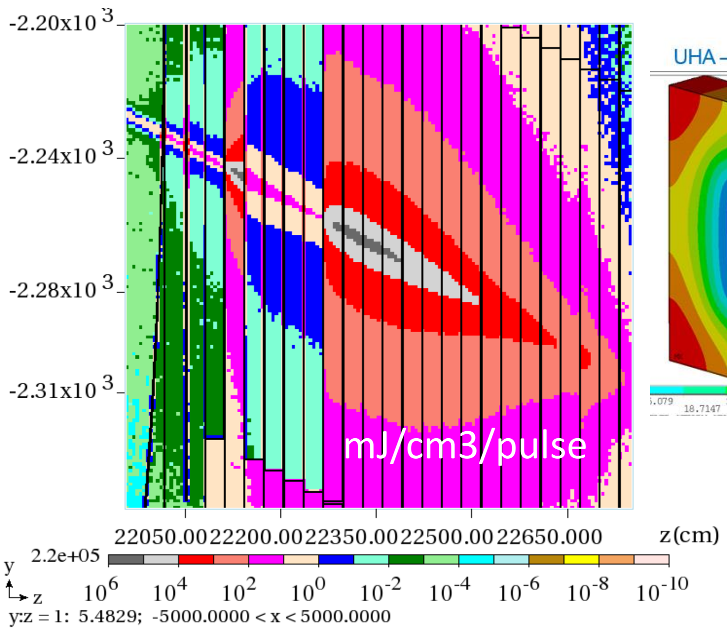


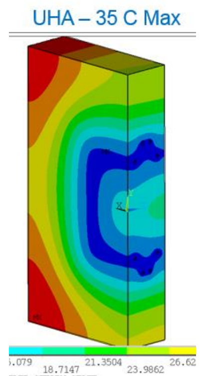




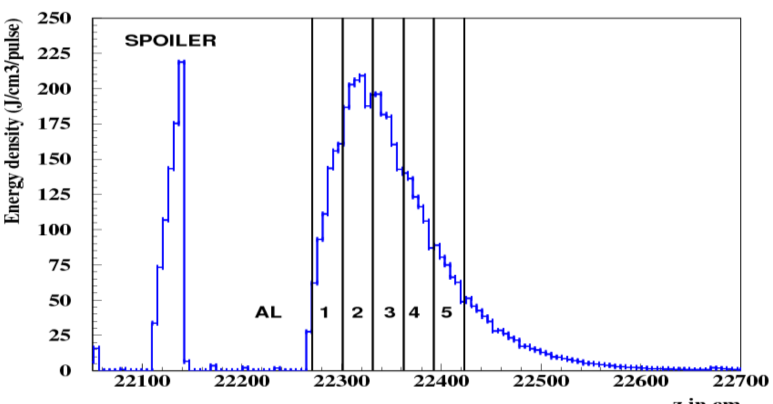
Hadron Absorber Complex: EDEP & Prompt Dose

No-target beam accident (σ=2.4mm)

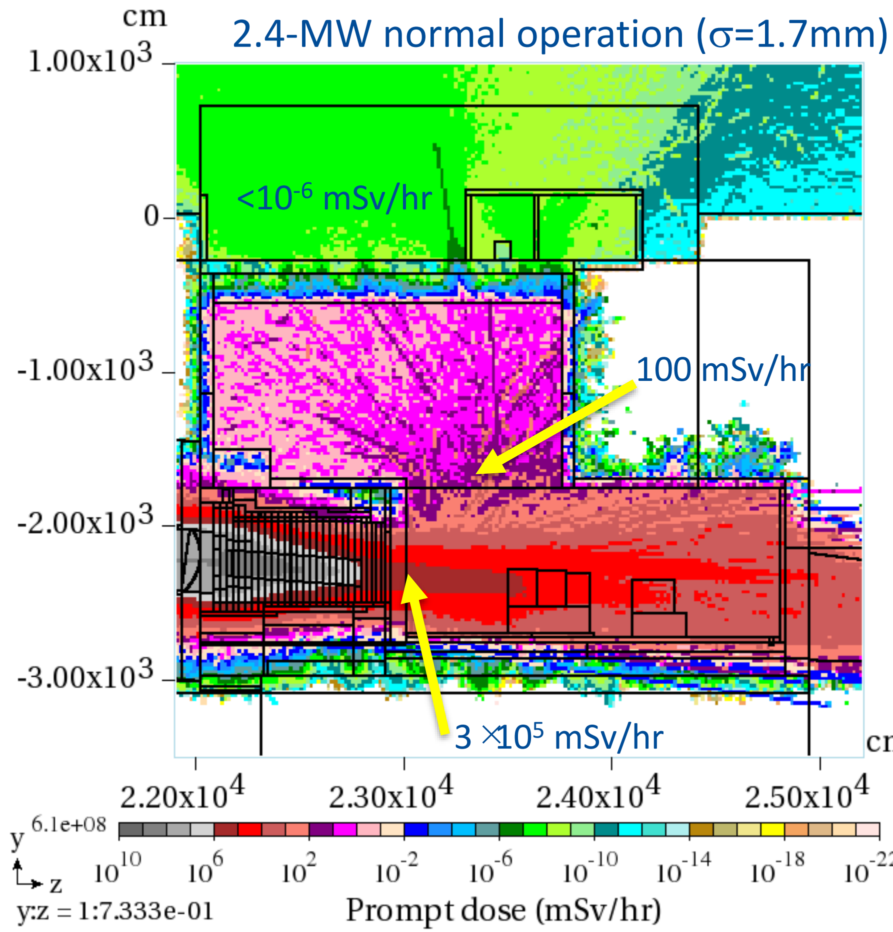




Temperature and stresses below the limits



2.4-MW normal operation (σ=1.7mm)



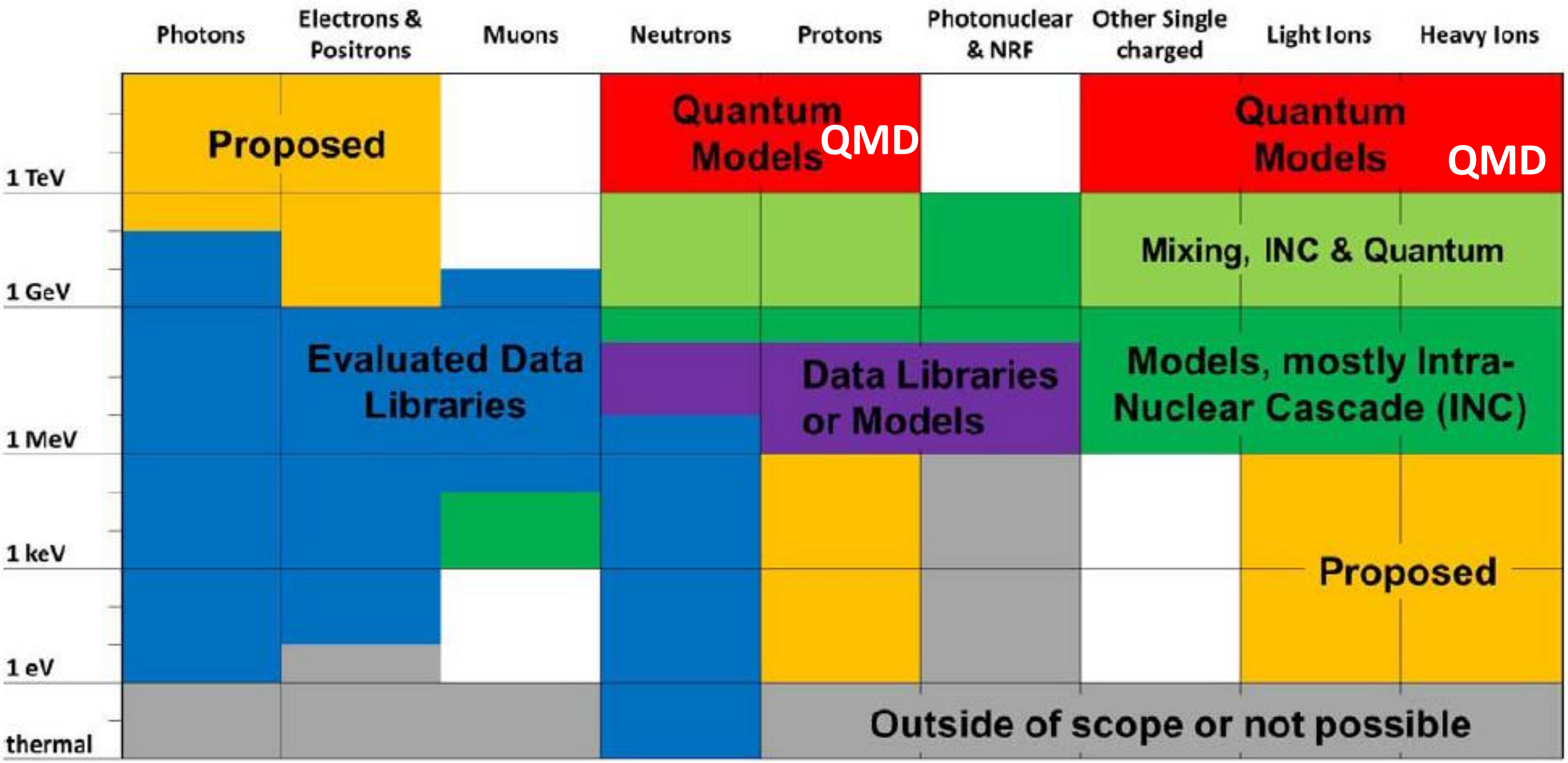
Carefully designed shielding guarantees prompt and residual dose, air and cooling water activation as well as radiation load on ground water to be below the administrative limits with corresponding safety margins

MCNP (mcnp.lanl.gov)

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for particle transport. ***MCNP is considered the industry standard for simulation in reactor, medical, space and low- and medium-energy accelerator applications.***

- Specific areas of application include radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, accelerator target design, fission and fusion reactor design, decontamination and decommissioning.
- The code treats an arbitrary 3D configuration of materials in geometric cells bounded by various surfaces.
- The neutron interaction and transport modules use standard evaluated data libraries mixed with physics models where such libraries are not available.
- MCNP contains a rich collection of variance reduction techniques.
- Important standard features that make MCNP versatile and easy to use include a powerful general source description, geometry and output tally plotters, a flexible tally structure, and an extensive collection of cross-section data.
  - For example, for neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B-VI) are accounted for.

MCNP Physics Models



MCNP Geometry, Magnetic Fields, Tests

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

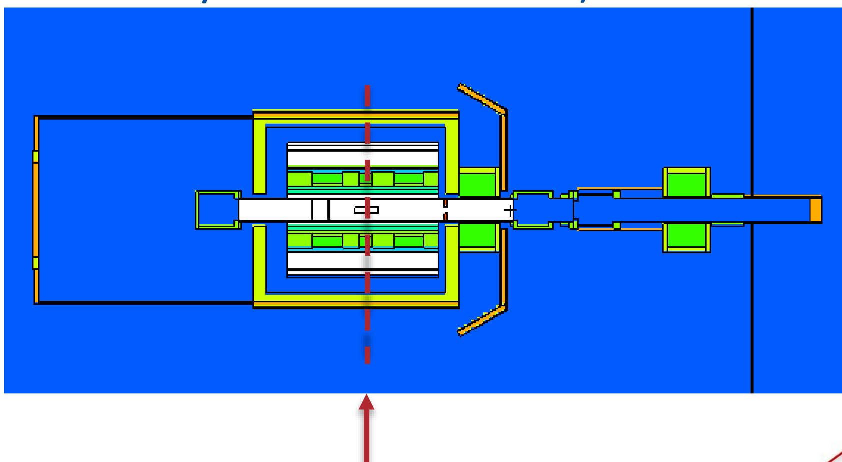
- Magnetic fields: (1) Constant dipole, square-edge quadrupole and quadrupole with a fringe-field kick – all in low-density materials, such as air; (2) COSY maps only in vacuum and specific to one particle type; both are rather limited compared to four other codes with the arbitrary EM field capability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

- **Unique feature:** MCNP 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 multitude of automated verifications, validations and regression tests. These tests are meant to detect any unintended changes to the code, and for installation testing.

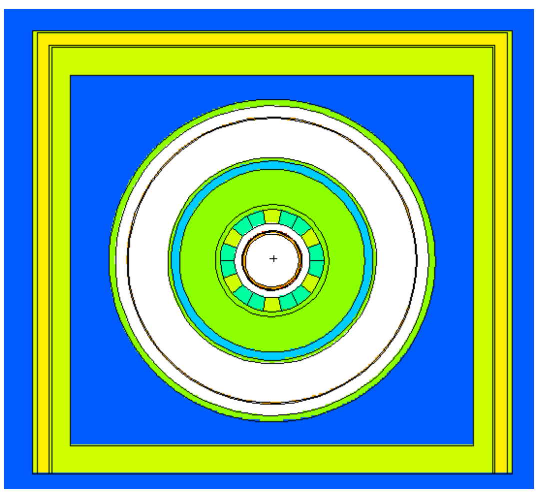
- Super-precise simulation of EMS at 1 eV to 100 GeV

MCNP Geometry & Tally Example

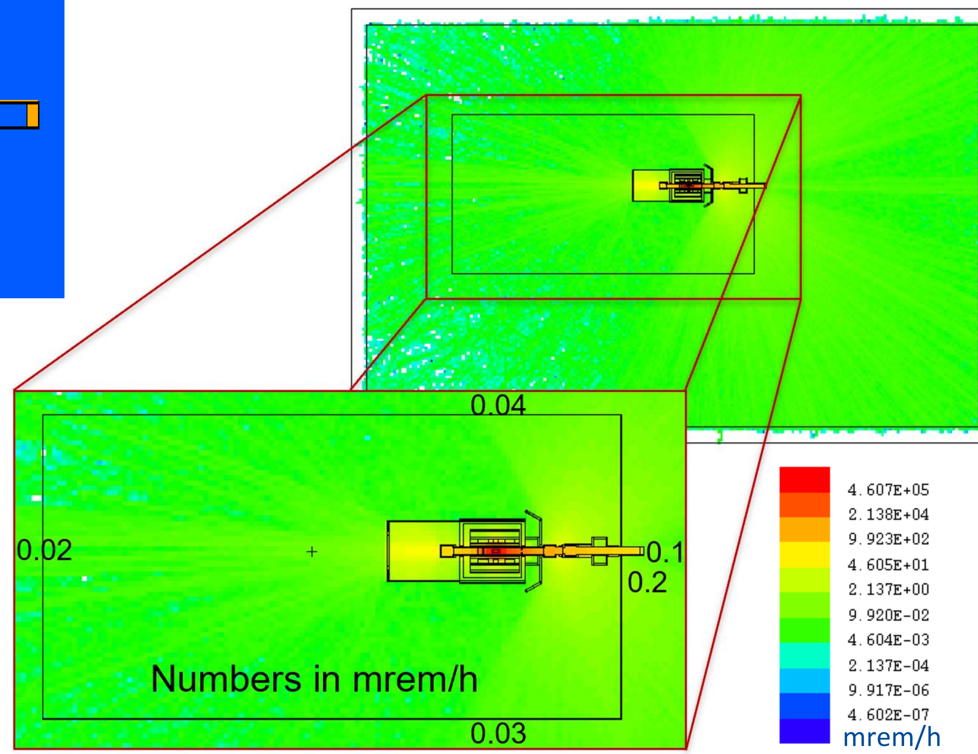
Geometry example: FRIB HP ECR (High Power Electron Cyclotron Resonance) ion source



Cross section view

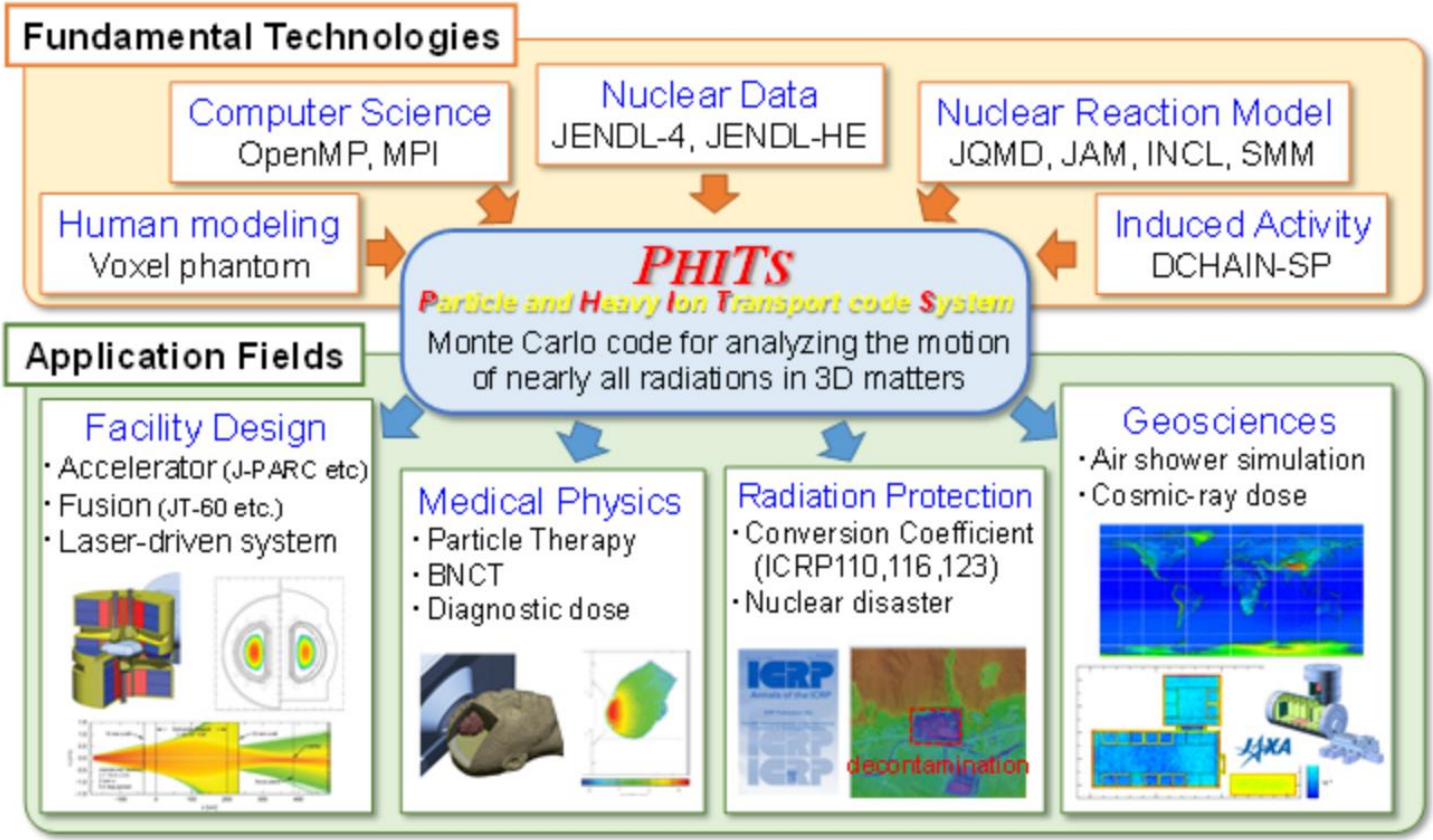


Tally example: prompt dose rate map



Fortran-90

PHITS (phits.jaea.go.jp)

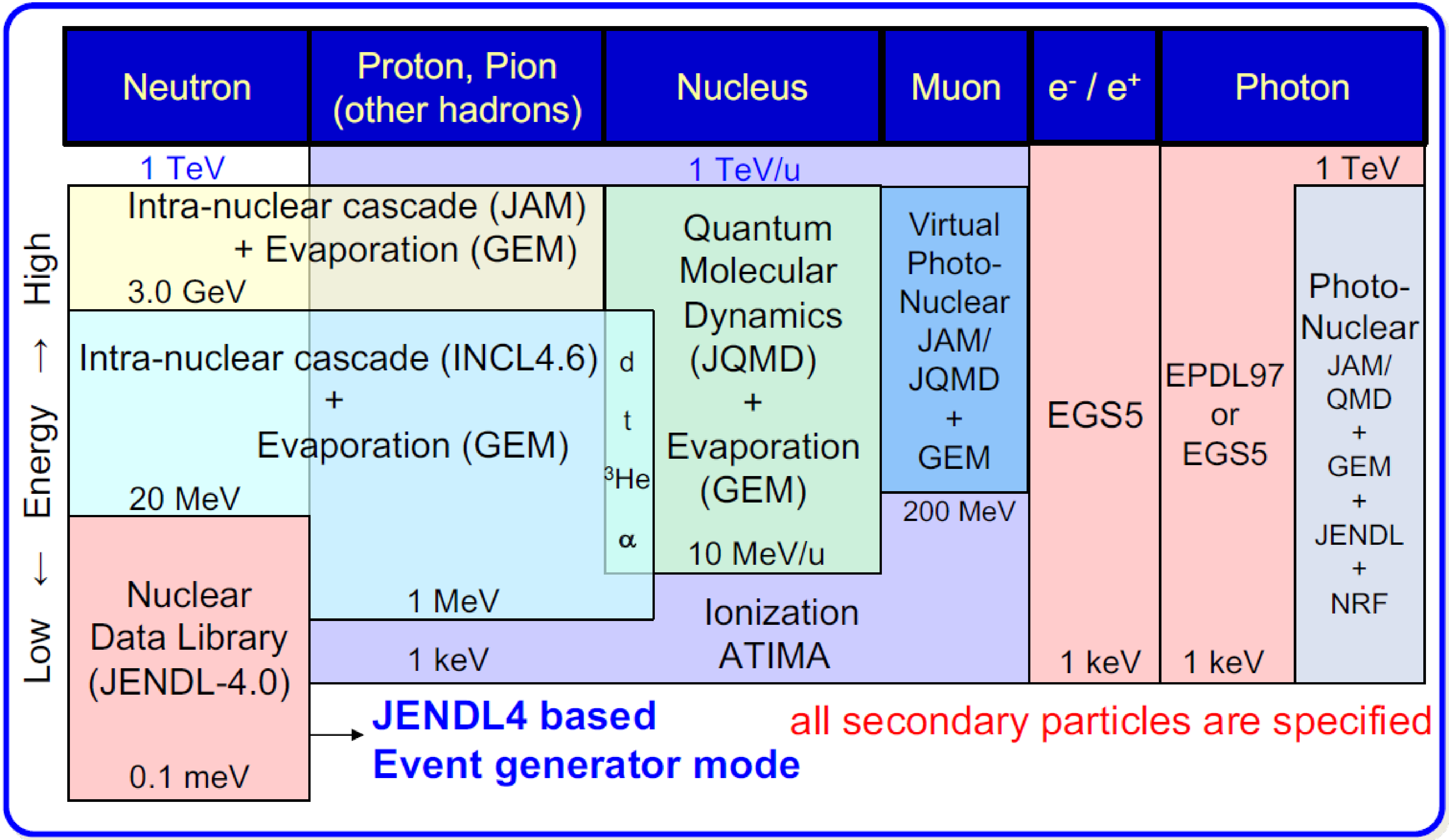


PHITS Features

PHITS 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 HE hadron transport code NMTC/JAM that was extended to heavy ions.

- Electromagnetic fields and gravity can be considered in transport simulation of all particles.
- The transport of LE neutrons employs cross sections from evaluated nuclear data libraries such as ENDF and JENDL below 20 MeV.
- 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.
- The time evolution of radioactivity is estimated using DCHAIN-SP module, a part of the code package.

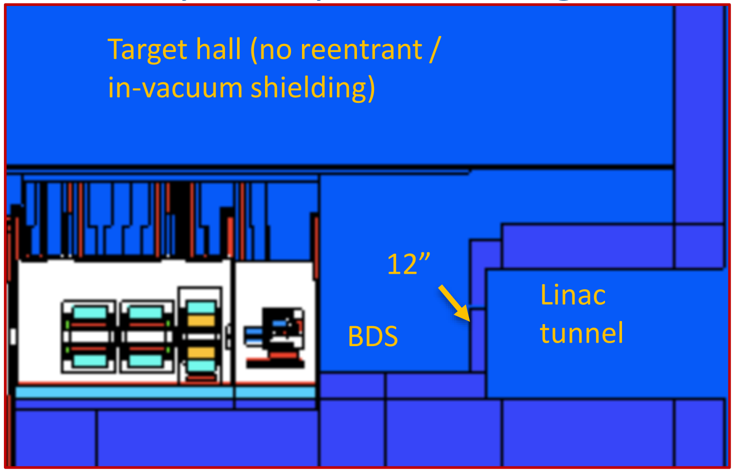
PHITS Physics Models



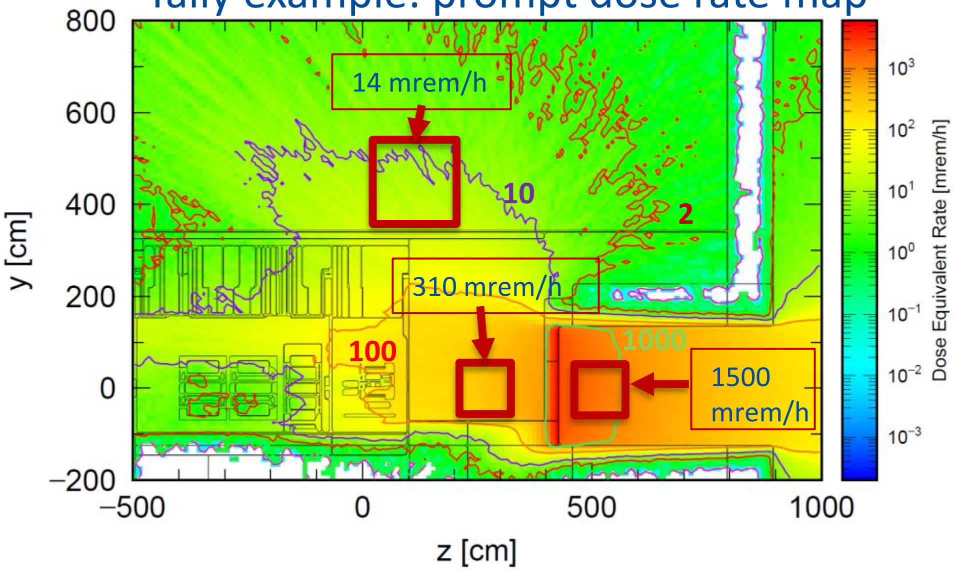
PHITS Geometry & Tally Example

- 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.

Geometry example: FRIB Target Hall



Tally example: prompt dose rate map



Code Benchmarking

- **Debugging:** The code should produce results consistent to what was expected to be produced
- **Validation:** Results should agree with established (analytical) result for the specific case
- **Intercomparison:** Two codes should agree if the underlying physics model is the same
- **Verification:** The code should agree with (reliable) measurements

CERN CHARM Facility at 24 GeV/c

T. Oyama et al. *Nuclear Inst, and Methods in Physics Research B 434 (2018) 29–36*

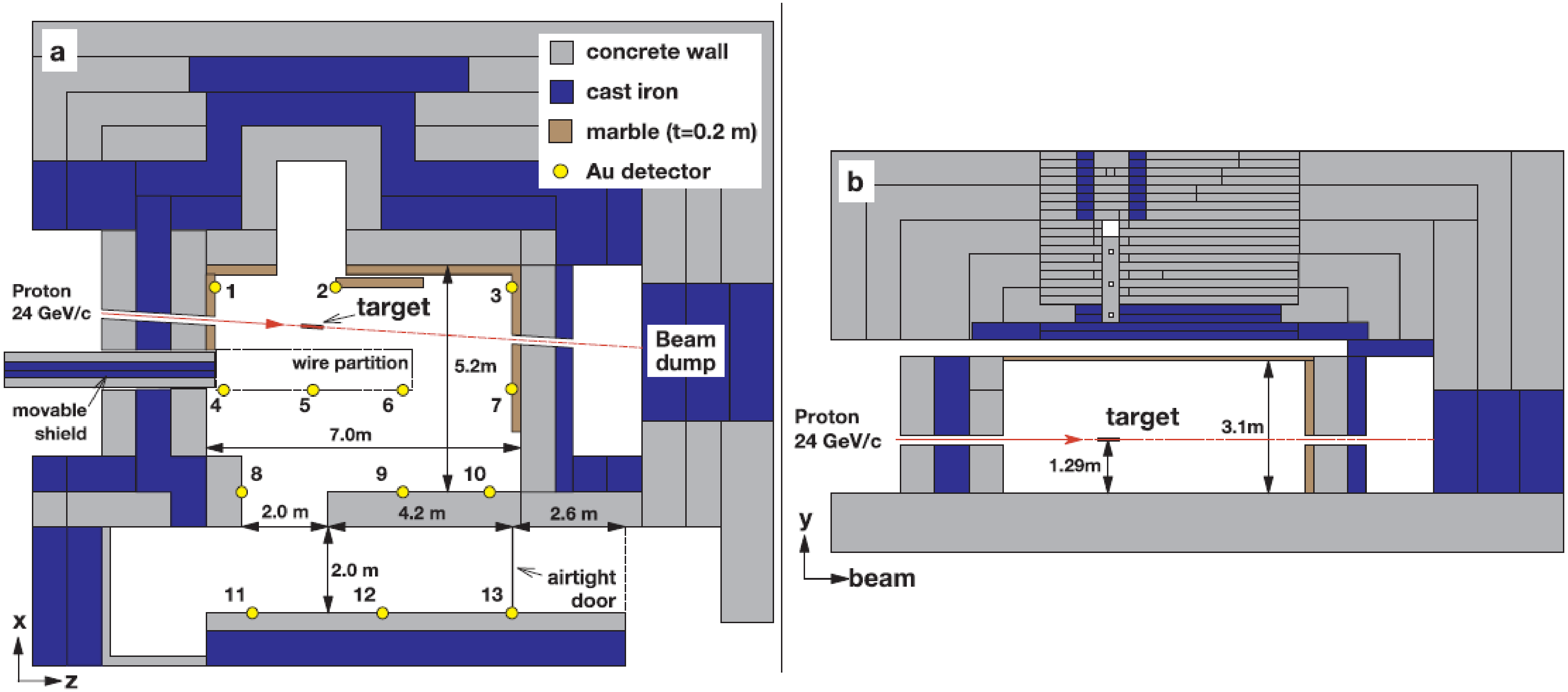
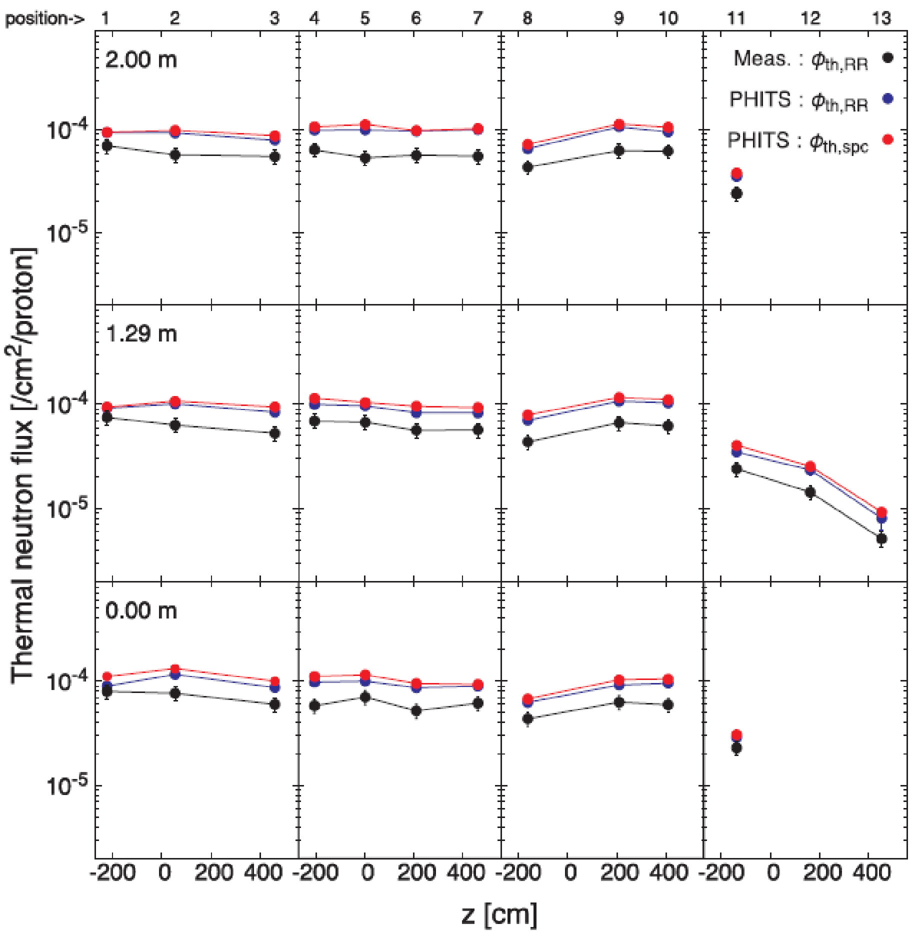
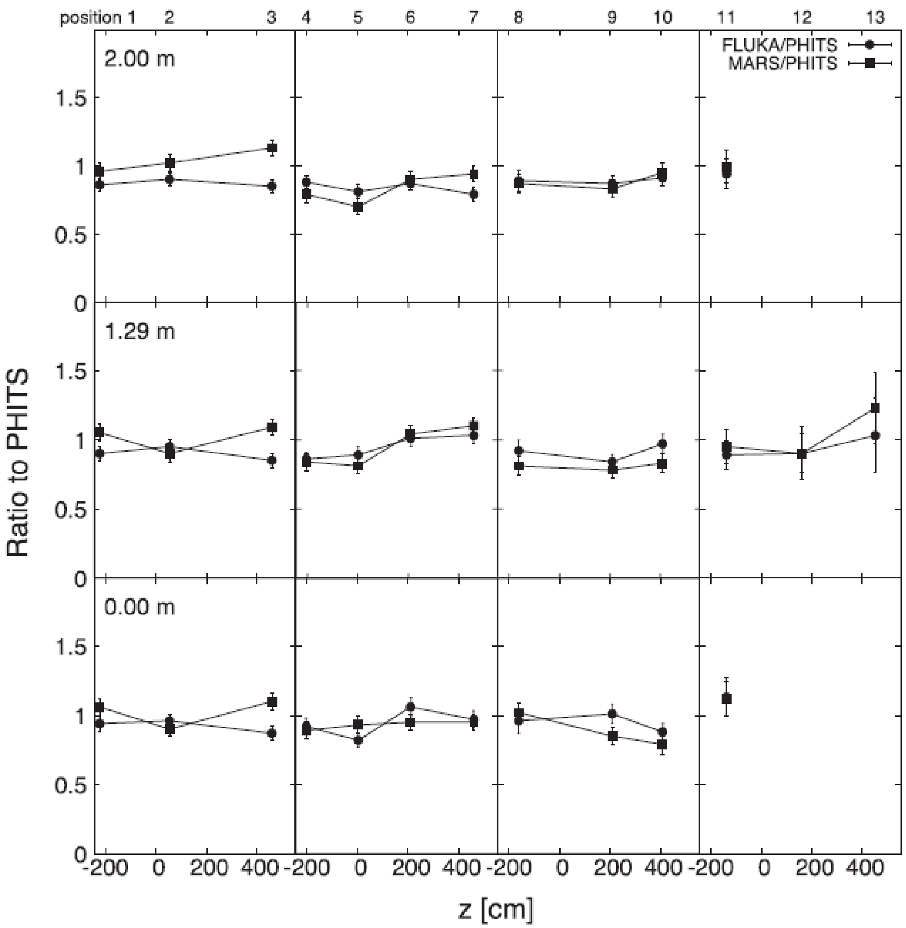


Fig. 1. Cross-sectional view (a) and longitudinal-sectional view (b) taken along the Cu target plane of the CHARM facility, together with important dimensions. The numbers 1–13 indicate the experimental location of the gold foils.

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

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Shielding and Radiation Effect Experiment

JASMIN Japan-FNAL Collaboration:

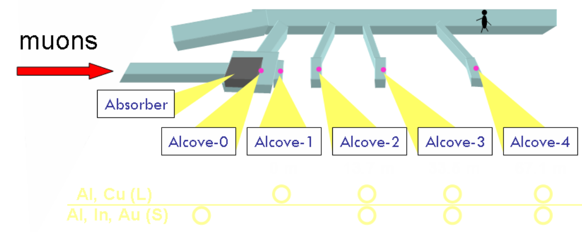
<u>Shielding and Radiation Effect Experiments at FNAL</u>

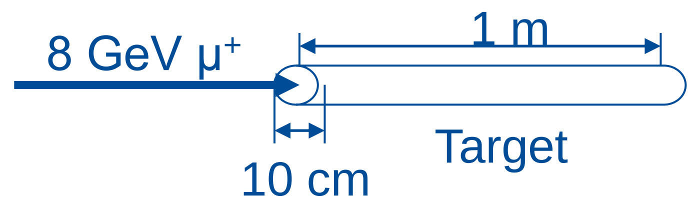
T-972 (2007-2009)

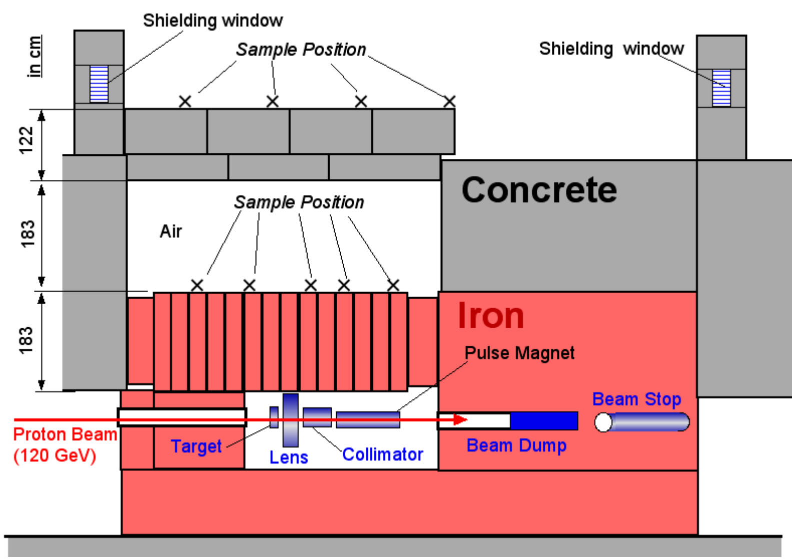
T-993 and T-994 (2009-2012)

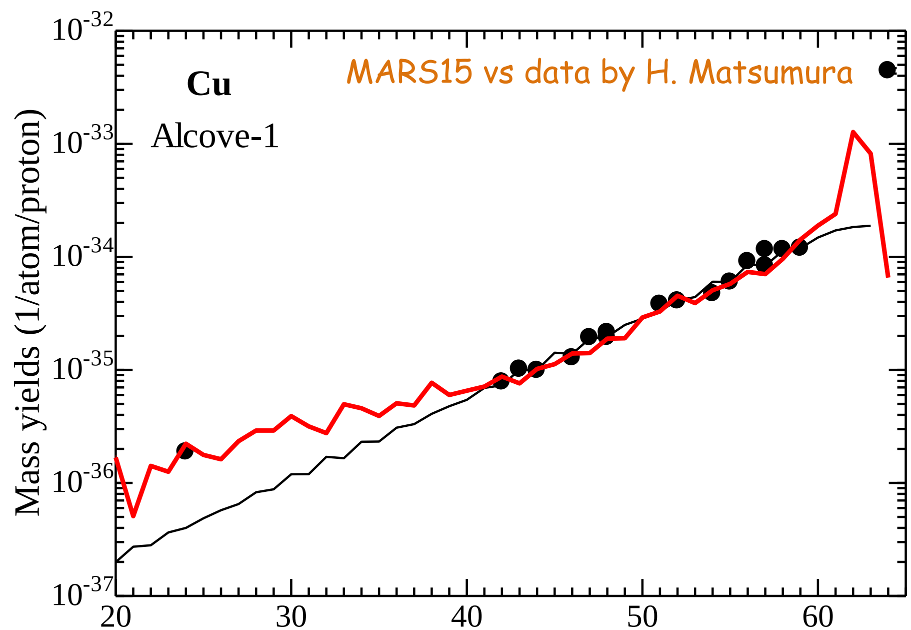
Shielding data and code benchmarking; targets, collimators and thick shields; radiation effects on instruments and materials

Example: Muon-induced nuclide production

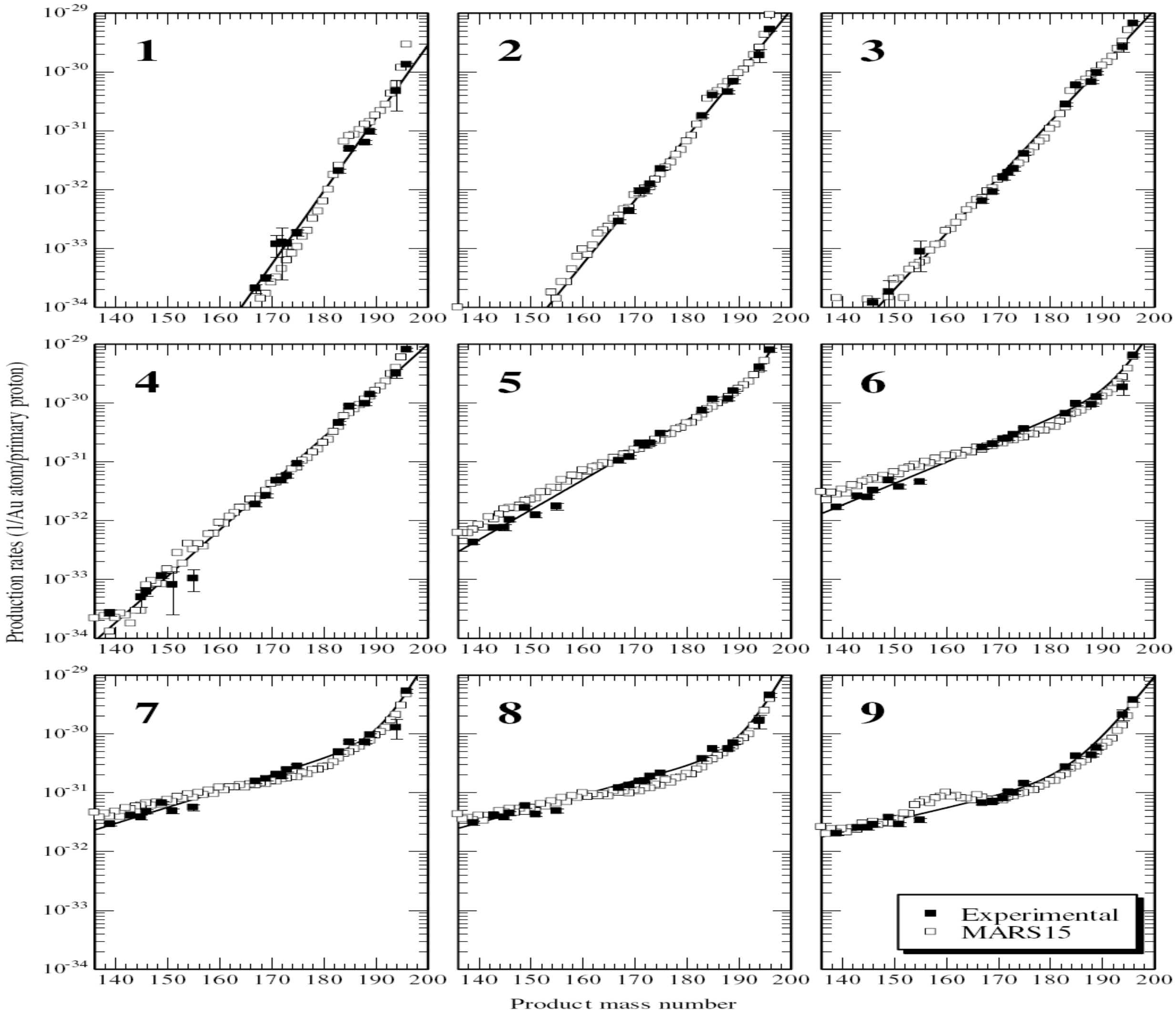


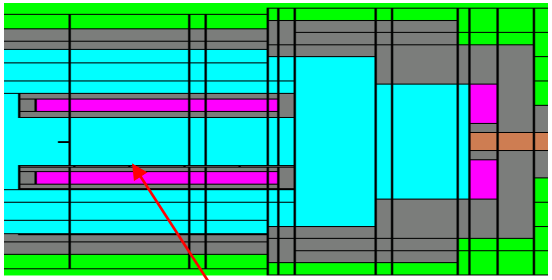


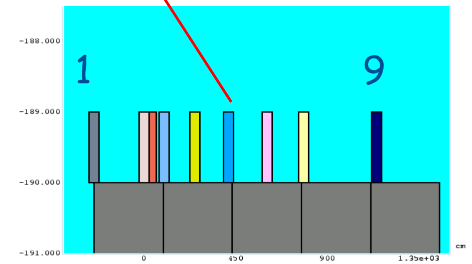




Nuclide Production at 12-GeV K2K Target Station







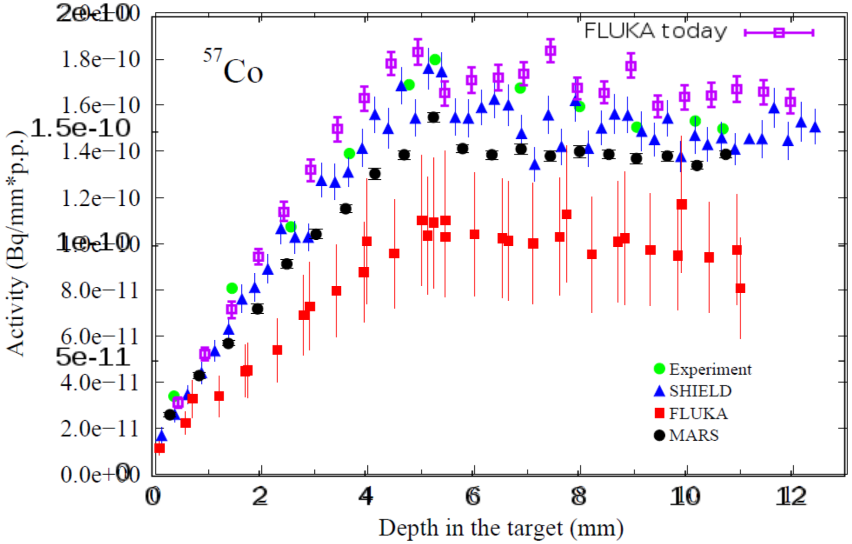
Nine gold foil samples over 12 meters

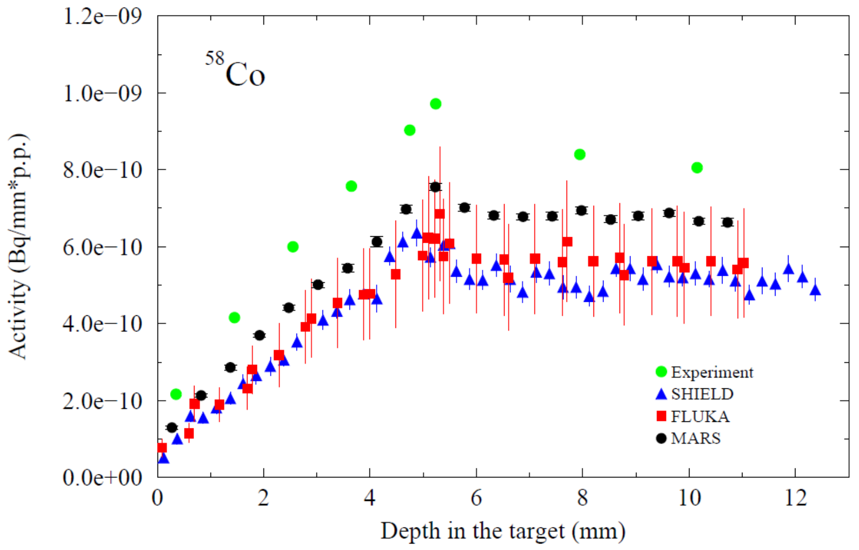
Fermilab

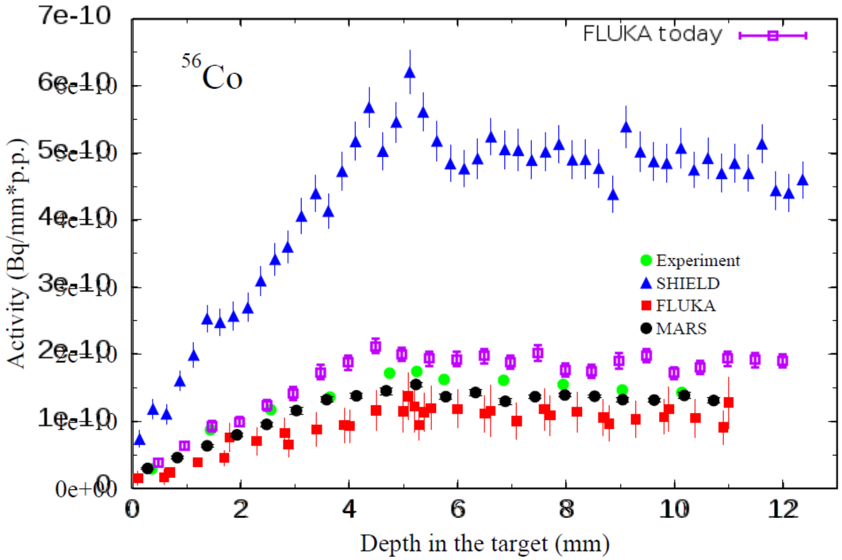
Activity Benchmarking at GSI

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

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







Air Activation at NuMI Neutrino Production Facility

To attain a higher 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 **B 414** (2018) 4-10

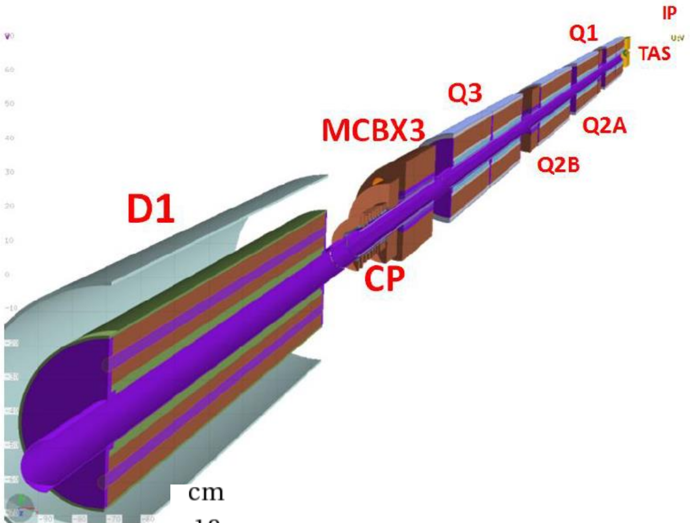
Measured and calculated production rate density (cm^{-3} POT^{-1} s^{-1}) for the most important radionuclides generated in the air in the beam enclosure of the NuMI target chase.

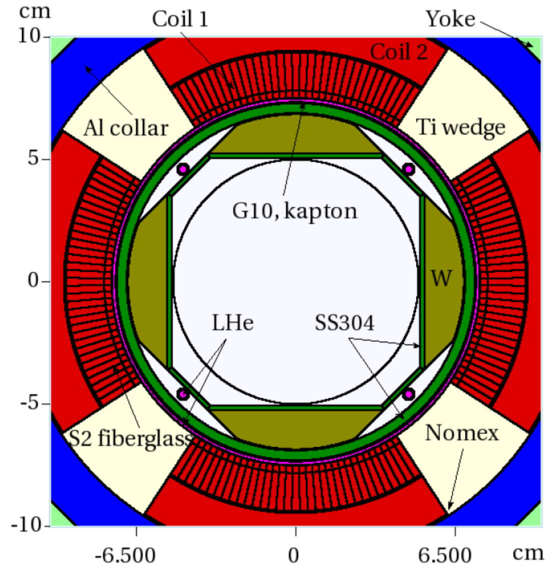
Production rate	^{41}Ar	^{11}C	^{13}N	^{15}O
Measurement	1.98×10^{-12}	6.38×10^{-11}	4.07×10^{-11}	3.50×10^{-11}
Standard methodology	6.85×10^{-12}	2.22×10^{-10}	5.22×10^{-11}	9.16×10^{-11}
MARS15	1.08×10^{-12}	4.44×10^{-11}	3.71×10^{-11}	4.16×10^{-11}
MARS15/data	0.55	0.70	0.91	1.19

50%

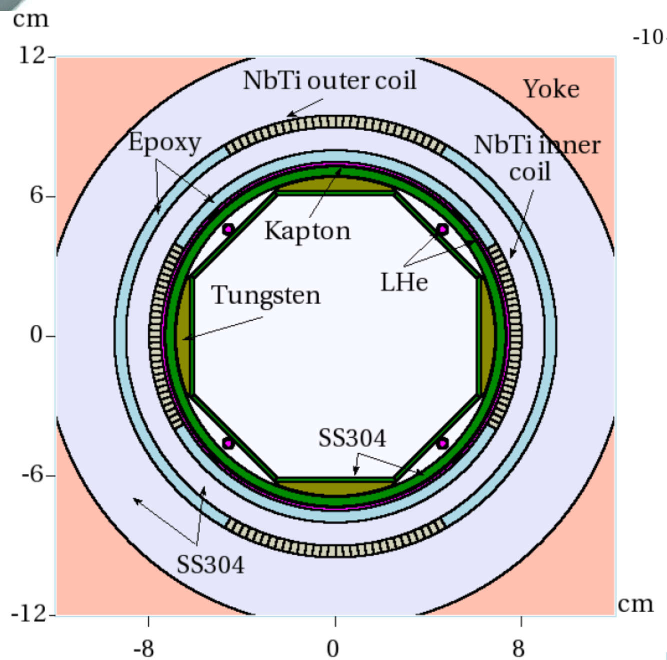
10-30%

HL-LHC IT FLUKA-MARS Study and Intercomparison



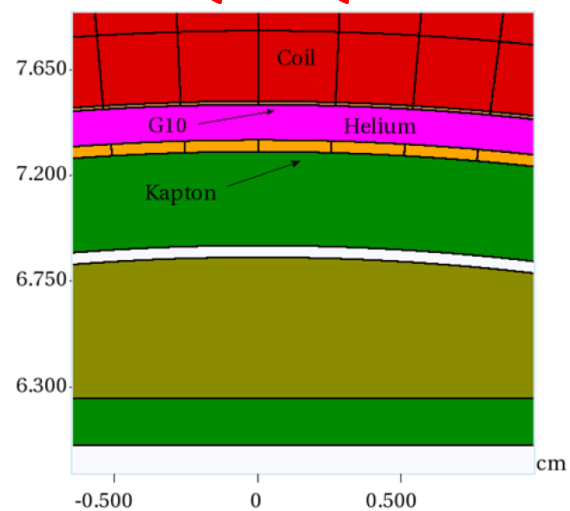


Q1



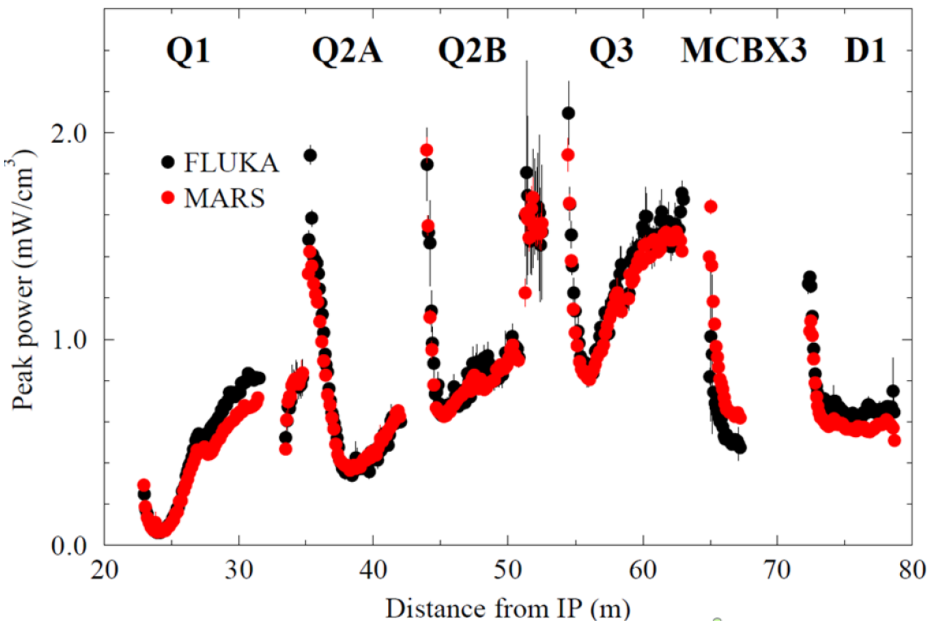
MCBX

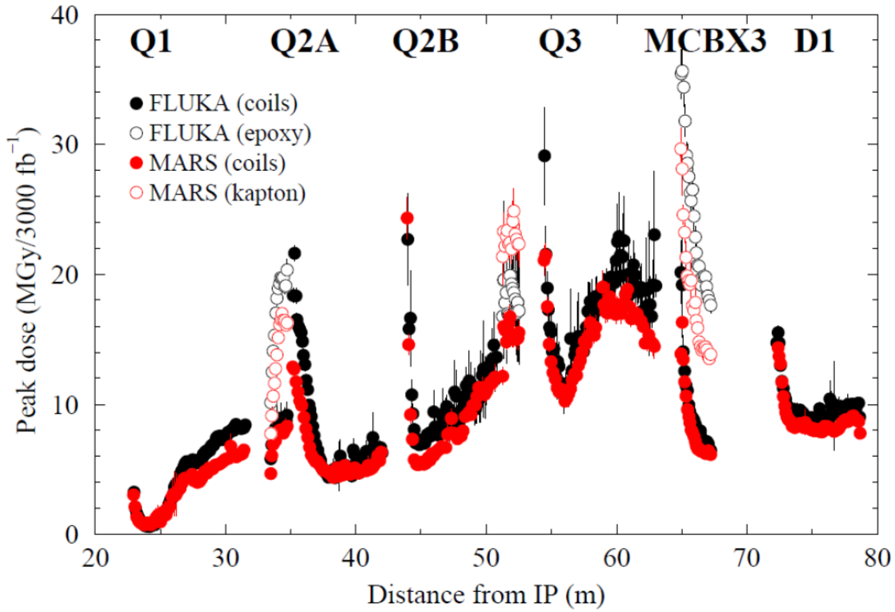
Q1-Q3 details



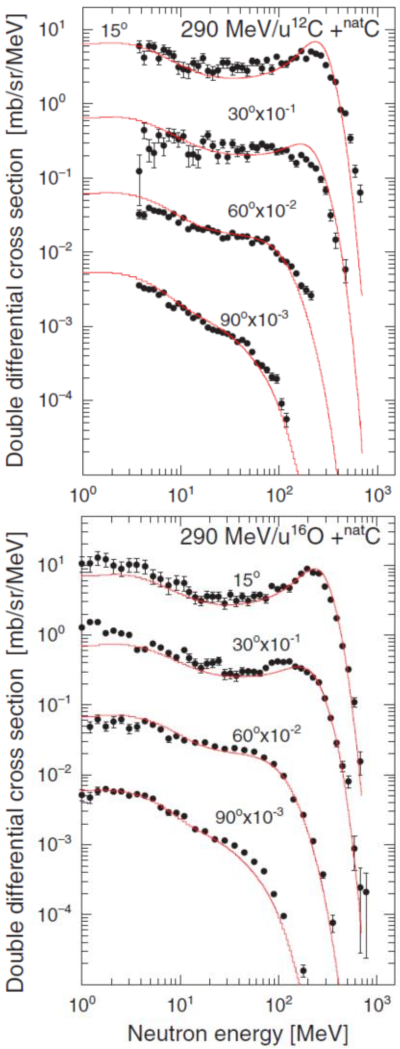
PRAB (2015)

HL-LHC IT FLUKA-MARS Study and Intercomparison





PHITS: Double Differential X-Sections & Neutron Production



Double Differential Cross Sections

Neutron production yields

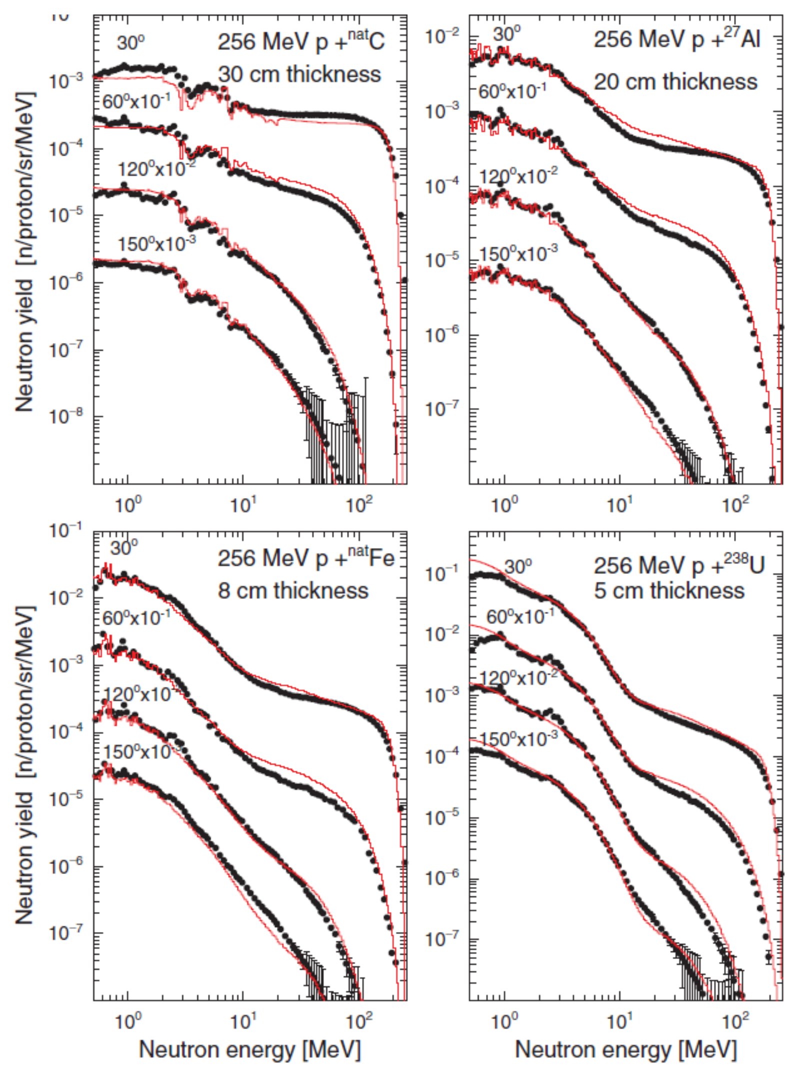
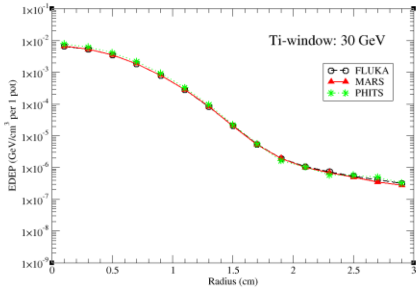
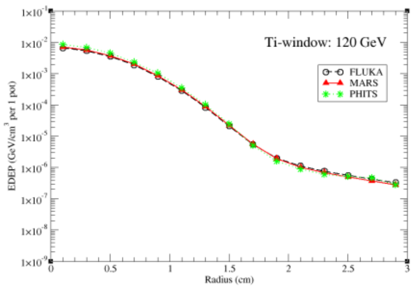
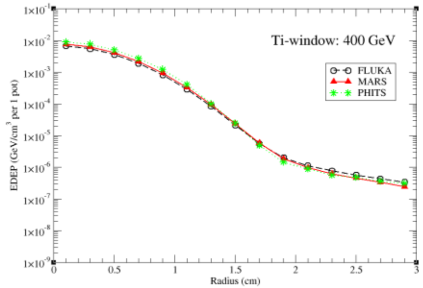


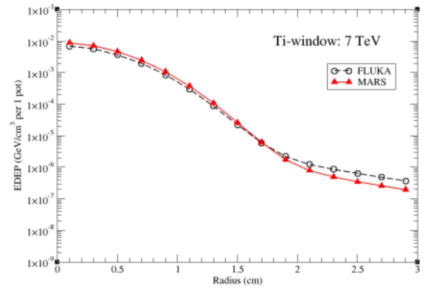
Figure 11. Differential neutron production yields at scattering angles of 30°, 60°, 120°, and 150° for an incident proton energy of 256 MeV on stopping lengths of C, Al, Fe, and U targets [33].

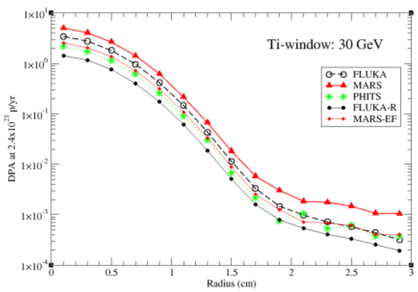
FLUKA, MARS, & PHITS: EDEP & DPA

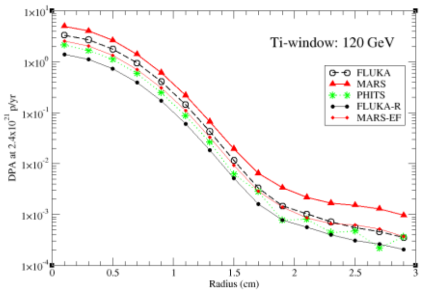


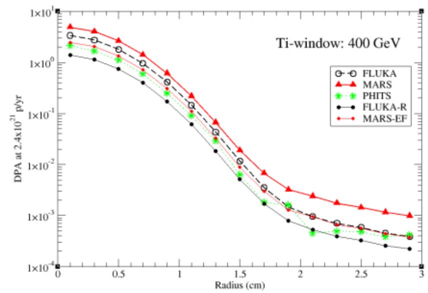


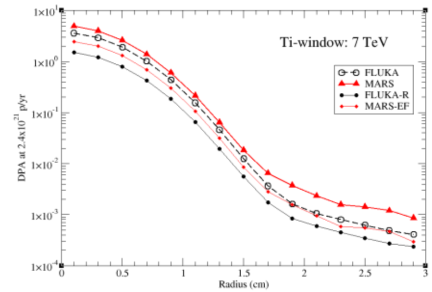












Summary

An overview of underlying physics in high-energy and/or high-power particle beam interactions with matter in accelerator applications and its implementation in the Monte Carlo simulations are presented and discussed. Effects in materials under irradiation, materials response related to component lifetime and performance are considered with a focus on existing and future accelerator complex needs.

The implementation of this multi-faceted physics and adequate state-of-the art computing techniques in the modern Monte Carlo codes, code main features, results of the code benchmarking, validation, and intercomparison are described.

MARS Group Post Doc Position Advertisement!

The MARS group in the Target Systems Department of the Accelerator Division at Fermilab is seeking candidates for a **Research Associate** position. The MARS code supports the laboratory's projects at all stages, from planning to operations and beyond. Demands for even more reliable and user-friendly MARS code complex are envisioned in the foreseeable future.

- The successful candidate would be a young physicist or nuclear engineer at early stages of their career, with good knowledge of particle and accelerator physics, modern computing and programming technologies, expert capabilities in code development, as well as experience in using high-level Monte Carlo particle-matter interaction codes such as FLUKA, GEANT4, MARS, MCNP, or PHITS. The primary function of the successful candidate will be to develop and support software, namely, Fermilab's in-house Monte Carlo particle-matter interaction code MARS. The successful candidate will be involved, together with the MARS group members, in the MARS code development, maintenance, modernization, and documentation. The candidate will be expected to work in a team environment and author technical documents and reports.

- The MARS group is involved in the design and upgrades of the high-power target, beamlines, collimation, absorber and experimental flagship facilities at Fermilab, such as LBNF, PIP-II, mu2e, as well as the MI-8, Delivery Ring, and Booster upgrades. The group uses the powerful computational tools to assess the radiation safety and efficiency of various approaches at each stage of a project. Having a strong team to keep the code up-to-date and working seamlessly is very important for achieving the lab's goals.

- Fermilab is America's premier laboratory for particle physics and accelerator research, funded by the U.S. Department of Energy.

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I would like to express my gratitude

- To Peter Ostroumov and my FRIB colleagues for their welcome …
- … To Nikolai Mokhov and members of his MARS group at FNAL for their support and guidance …
- … And to you all for your attention!

Contact email: dgeorgob@fnal.gov

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