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Simulation of ion propagation in the microbeam line of CENBG using GEANT4

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Abstract

For more than five years the use of microbeam setups for the irradiation of biological samples has opened a new field of investigation in the study of radiobiological effects at low doses. Since 1998, a single ion irradiation system has been developed on the microbeam line of CENBG. Compared to the already existing systems, based on collimated beams, the use of a focused microbeam gives the advantage of a faster irradiation procedure, since the beam can be positioned onto the targeted cells by means of a fast electrostatic deflection system. Single cells irradiation requires a precise control of the position of the incident ions on target, with a spatial resolution of a few microns. All the components of the microbeam line must be designed in order to minimize the spatial dispersion of the beam: single ion transmission detector, collimators used along the beam line, exit window... To understand and to control the different processes of ion diffusion which can occur all along the beam line is thus a crucial point. For this, a reliable beam transport simulation tool is required. For more than 20 years nuclear physicists have used the GEANT code to simulate particle–matter interaction. Its most recent version, GEANT4, with an object-oriented architecture, allows to simulate different components of a beam line, considered as objects that can be inserted into the code. The beam line and the detectors geometry can be easily implemented. Moreover, the simulation code can be interfaced with computer-assisted design systems and numerical analysis software packages. In this article, the first attempt to use GEANT4 to simulate components of a microbeam line with protons and alphas of a few MeV will be presented.
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1. Introduction

The Monte Carlo code GEANT was first developed in FORTRAN at CERN to simulate particle–matter interactions [1]. The new GEANT4 project [2] came up in December 1994. GEANT4 is a freely available object oriented code, written in C++, allowing complete flexibility, extensibility and interactivity with external software (data storage and analysis, computer-assisted design, ...). All physics processes, models and visualization modules are entirely accessible to the user. The code is documented with manuals, examples,

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and experts are available for support. The last version (version 4.1 plus patch 01, released on 07/31/2002) includes very low energy electromagnetic processes [3] (down to tens of electron-volts) to extend the use of GEANT4 to space physics and to medical physics. This allows us to propose for the first time the development of a simulation package of the CENBG microbeam line.

In this simulation package, the main program constructs a run manager object, like in any GEANT4 application, which controls the whole simulation process. According to the user's needs, several classes must be implemented to describe the experimental setup construction (materials used, beam line element geometries, detector sensitive components, magnetic and electrical fields, ...), the primary particle generator (primary beam characteristics, such as particle type, kinetic energy distribution, position distribution, direction distribution, emittance, ...), the list of particles that can be generated by the simulation and all the associated physics processes [4].

The simulation package has been developed at CENBG on a dedicated Pentium 4 personal computer running Linux RedHat 7.2 [5] with the gcc compiler 2.95.2 installed, where the last version of GEANT4 and its low energy extension have been installed. It has been entirely interfaced with the C++ data analysis environment ROOT [6] (data storing, histogramming, fitting, ...) developed and available freely at CERN. OpenGL and VRML drivers have also been installed for online visualization of the simulated interactions.

2. Validation of GEANT4 at microbeam scale

A study of GEANT4 and its low energy extension performances was performed at micrometer scale to validate the simulation package with experimental results. We have reproduced the experimental setup used to measure the lateral straggling of the CENBG microbeam as described in [7]. A proton or alpha beam with a kinetic energy of 2.5 MeV was delivered on polymer Mylar (formula $C_{10}H_8O_4$, density 1.397 g/cm^3) foils of different thicknesses, placed in the focus plane of the microbeam lenses. The lateral spreading of the beam was measured 6.3 mm after the foil, using a silicon charged particle detector collimated down to 10 μm. The measurements were also compared to the Monte Carlo predictions of the simulation code SRIM 2000 [8]. GEANT4 predictions for the beam full width at half maximum (FWHM) as a function of foil thickness are shown on Fig. 1 for a proton beam and alpha beam, along with a third order polynomial fit to experimental measurements and a third order polynomial fit to SRIM 2000 predictions. The beam FWHM was obtained from the standard deviation σ (FWHM $= 2.354\ \sigma$) of a gaussian fit – performed with ROOT and the minimization code MINUIT – to the beam spread measured 6.3 mm after the foil. The horizontal error bars on GEANT4 predictions take into account a $\pm 5\%$ experimental uncertainty on the foil thickness value and the vertical error bars combine statistical fluctuations obtained by varying the number of incident particles in the simulation and systematic fluctuations of the FWHM values due to the $\pm 5\%$ error on the foil thickness; they range from 1% to 4% for protons and from 5% to 7% for alphas. The default "ICRU R49p" (He) electronic stopping power tables have been used for protons (alphas) in the implementation of the low energy ionisation process for charged particles, as can be specified by the user. The "Ziegler 1977p" (He) tables have also been used and show compatible results. The GEANT4 4.1 predictions show a good and stable agreement with experimental results over the range of measured thickness, giving us more confidence in this new simulation tool at the micrometer scale.

3. Simulation of CENBG beam line components with GEANT4

The oriented object structure of GEANT4 allows the user to define his own classes, derived from the GEANT4 virtual classes. One class can be defined for each beam component, such as collimators, quadrupole magnetic lenses, ... They can be combined together to build the entire beam line setup. We present below the study of beam

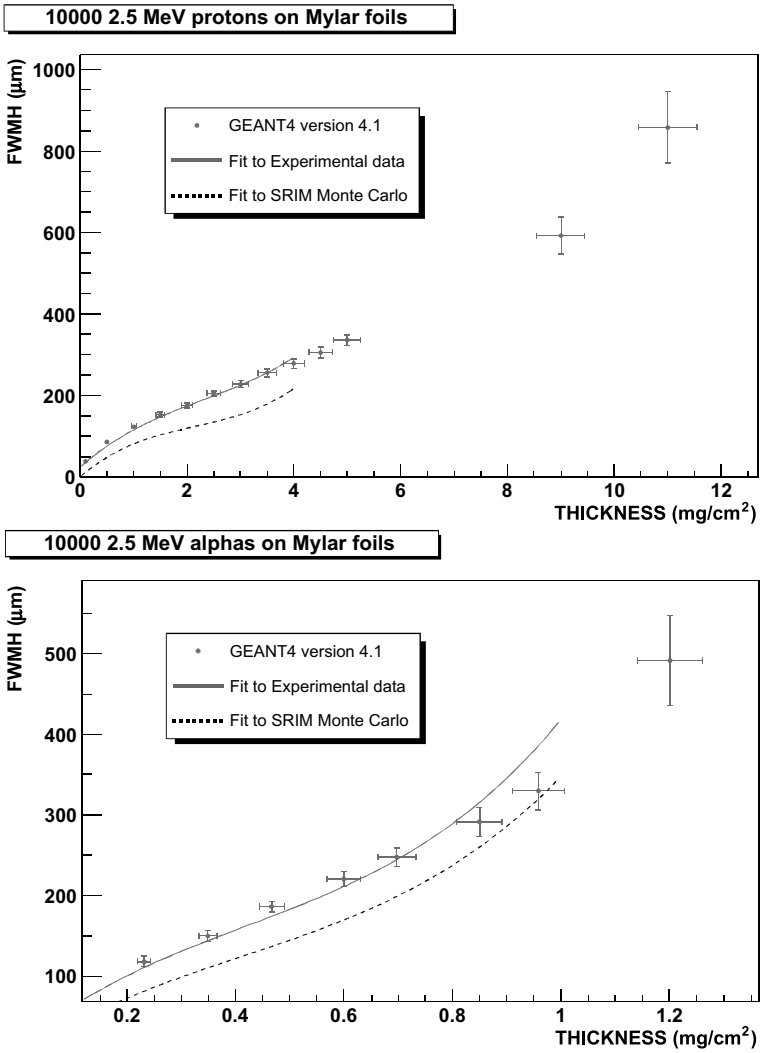


Fig. 1. Simulation of beam straggling. See text for details.

propagation and scattering through circular collimators, magnetic focus lenses and the extraction of the beam back into the air.

3.1. Collimators

Collimators can be built applying Boolean operations to basic geometrical volumes available in GEANT4, for example, a simple circular Platinum collimator can be designed by subtracting a cone to a Platinum parallelepiped box with a thickness of a few microns. The main difficulty lies in the determination of the physical dimensions of the collimator itself that needs to be reproduced within GEANT4. Observations of the collimator dimensions using an optical or an electronic microscope are often not sufficient to measure precisely the actual dimensions in the three dimensions, but can provide rough estimations that can be entered into the simulation.

As an illustration, we have reproduced the scattered energy profile of a 2.8 MeV proton beam through a circular Platinum cone of 10 μm. The primary proton beam energy and position

distributions were assumed to be gaussian, with a standard deviation of respectively 3 keV in energy and 0.425 μm in position on both vertical and horizontal axis, leading to a beam FWHM of 1 μm. The beam was swept on a square 128×128 node matrix of 46×46 μm side to cover the whole collimator aperture. The optical and electronic microscope observations of the collimator revealed the existence of a blurred "double cone" like structure. This geometry was implemented in the simulation code. Fig. 2 shows the 3-D distribution of the scattered energy as a function of the vertical and horizontal position of the incident proton when hitting the collimator. This distribution reproduces nicely the collimator profile. Experiment and simulation show qualitatively close scattered energy distributions, as long as the detector energy calibration is known with sufficient precision. However, the experimental distribution of the scattered energies presents discontinuities, revealing the existence of irregularities within the thickness geometry, probably created during the laser drilling of the collimator. These irregularities were not seen during microscope observations and consequently were not taken into account by the simulation. Nevertheless, the easiness of geometry design within GEANT4 makes it an ideal tool to study various collimator and slit geometries (Nobiling type for example) in order to reduce the beam scattering. More complex geometries designed with standard CAD tools can in any case be read and implemented by GEANT4.

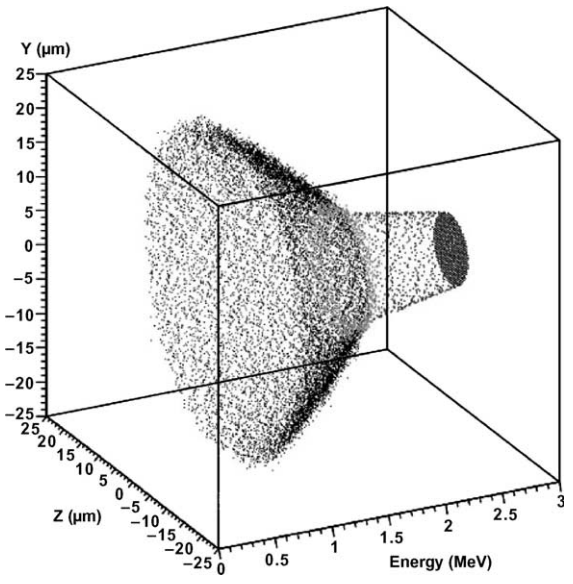


Fig. 2. Simulation of a 2.8 MeV proton beam through the circular collimator described on Fig. 2. See text for details.

3.2. Magnetic focus lenses

GEANT4 can deal with electrical and magnetic fields and knows how to integrate a particle motion equations, allowing the user to track down every particle when propagating through the field. It uses by default Runge Kutta 4 integration method and only needs to know the field three components at each point (x, y, z) of the simulated volumes. A magnetic field can be given as an analytical expression or by a dedicated method reading a magnetic map.

The four focusing quadrupoles of the CENBG microbeam line have been simulated knowing precisely their geometrical sizes, their position along the beam line and their quadrupole field gradient. A 8 MeV proton beam (or, equivalently, a 2 MeV alpha beam) is generated 6 m upstream with a gaussian transverse position distribution of standard deviation 4.25 μm (corresponding to a beam FWHM of 10 μm), a gaussian energy distribution of 8 MeV (standard deviation 4 keV) and a uniform angular size of 0.5 mrad around the beam propagation axis (x). Consequently, the aperture of the first quadrupole is limited by ± 3 mm. Each quadrupole has an effective magnetic length of 15 cm inside a cylindrical tube with a 1 cm radius, and is separated from its neighbour by 4 cm. The focus configuration adopted is the so-called Russian configuration (focusing–defocusing, F–D), with the following gradients: 5.8928 and 14.6466 T/m, to achieve an overall focus of 10/1. The trajectories of the focused beam have been recorded during the simulation every 100 μm, to allow a precise determination of the position of the vertical and horizontal focus transverse planes along the line. The simulated beam profiles follow nicely the expected ones and are shown on Fig. 3 for a sample of 100 protons. Vertical and horizontal focus planes are located 230.15 ± 0.05 mm downstream the last quadrupole. Due to the

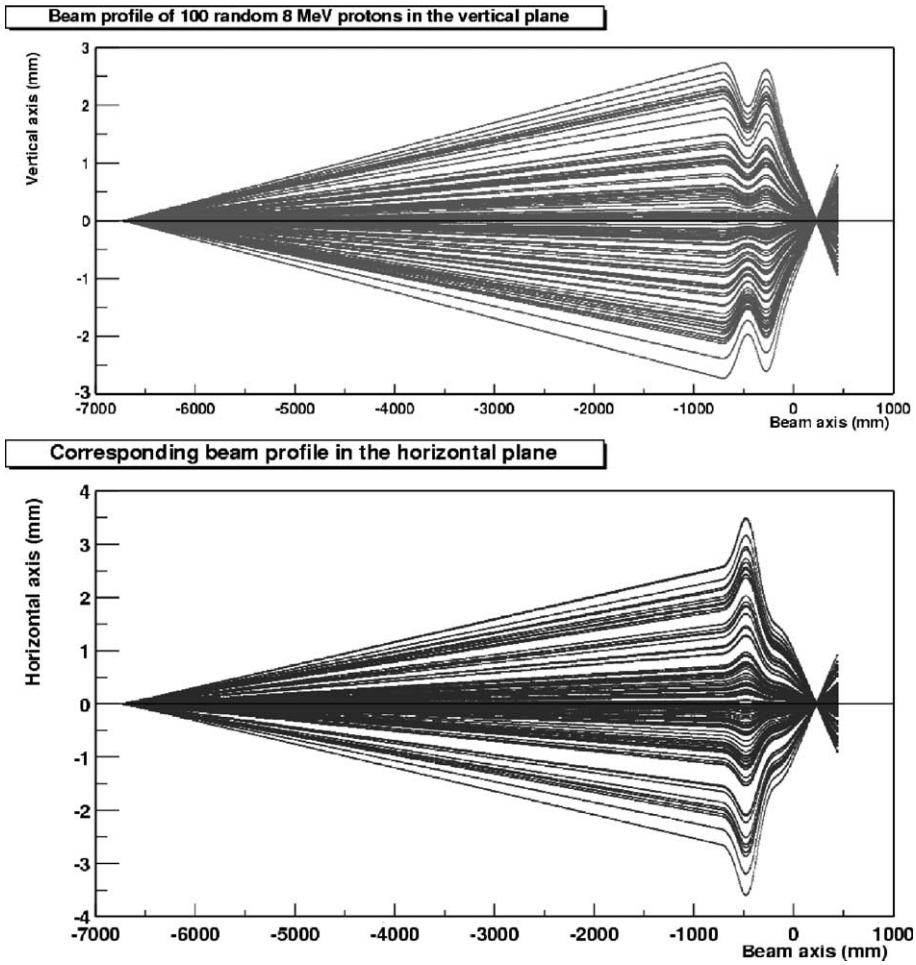


Fig. 3. Simulation of a 100 proton beam of 8 MeV through the four magnetic lenses of the CENBG microbeam line. Details in the text.

gaussian energy and position distributions of the incident beam, the beam position distribution in these focus planes – for the vertical transverse distribution – is close to a gaussian distribution with a standard deviation of 0.55 μm, corresponding to a FWHM of 1.3 μm. With a beam energy standard deviation of 4 keV, the global focus factor is, as expected, of order 10/1.3. More advanced studies could be performed by defining carefully the emittance of the beam (distribution of momentum versus position along the transverse y and z axis) at the emission point and by following its evolution through the magnetic lenses. Magnetic field leaks close to each quadrupole entrance and exit could also be introduced as long as they are well defined. Various geometry changes could be applied to each individual component, like tilts, to estimate their impact on the beam spread in the focus plane, where the targeted cells are placed.

3.3. Beam extraction

In order to irradiate living cells with a counted number of particles, a beam extraction stage has been inserted on the microbeam line of CENBG. The design of this stage is described in [9]. For the control of the beam, two detectors were developed: a thin scintillating foil (BC400®, 7 μm) for a proton beam and a low pressure gas detector (Isobutane, 5 mbar) for an alpha beam. Before hitting the

cells, the particles interact with different materials: the transmission detector material, possibly a silicon nitride exit window for alpha particles, a residual air layer and the cell culture support. A good description of the beam modifications due to this part of the beam line, especially angular scattering, should help us to improve the setup performances. As they present a simple geometry, both detectors can be easily implemented in GEANT4. The entire beam extraction stage can be described by adjacent parallelepiped boxes filled with the appropriate material (BC400®, Isobutane, Si_3N_4, air ...). Since the beam scattering predictions given by GEANT4 at the microbeam scale (see Fig. 1) seem to agree with experimental data, the next step of the study will be to obtain an estimation of the characteristics of the beam (position distribution, energy distribution, ...) when reaching the targeted cells.

4. Conclusion

The first studies presented in this contribution give better confidence and open new perspectives in simulations at the microbeam scale with GEANT4. They contributed to substantial corrections performed during Spring and Summer 2002 on the official multiple scattering and low energy ionisation modules developed by the GEANT4 collaboration.

GEANT4 is today the only all-inclusive beam line simulation tool written in C++ taking into account physical processes, from primary particle generation, ray tracing, to signal digitisation. Several subatomic physics groups are now improving GEANT4 capabilities at the physics–biology frontier, working in cooperation with biologists and physicians. We believe that constant evolution and development, as well as worldwide debugging by independent experimental groups, will contribute to make GEANT4 one of the most reliable simulation code.

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