USING GEANT4-BASED TOOLS TO SIMULATE A PROTON EXTRACTION AND TRANSFER LINE

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Abstract

The simulation toolkit GEANT4 has been used to create high-level tools for specific user groups, such as SPENVIS in space physics and GATE in medical imaging. In Accelerator Physics, comparable efforts are being devoted to develop general-purpose programs for simulating beam lines and accelerators, allowing access to Geant4's facilities for 3D geometry, tracking, and interactions in matter without the need for specialised programming techniques. In this study we investigate the use of two high-level tools based on Geant4, BDSIM and G4BEAMLINE, to model a 65-meter beam line supplying protons from the TRIUMF cyclotron to the ISAC Rare Isotope Beam facility. We outline some features of the codes and comment on their different approaches to defining the beam line geometry. Due to its ability to model some important aspects such as rectangular dipoles and magnetic fringe fields, G4beamline was utilized for the simulations presented here, for validation of the model and the investigation of beam losses.

INTRODUCTION

In using simulation tools to investigate particle losses in accelerators and beam lines, the effects of particle interactions in matter, and in particular the secondary particles arising from electromagnetic and hadronic interactions, are very important for safety issues, loss monitoring and diagnostics, and radiation damage and activation of hardware.

The Geant4 simulation toolkit[1] offers a versatile way to track particles in an accelerator or beam line geometry, with realistic fields. For interactions in matter it offers a wide range of physics processes and models and a host of other facilities for studying losses with tracking of all relevant secondaries. The choice of physics models allows tuning of the simulation to the particular energy range and particles of interest.

Tapping into the power of Geant4 generally requires facility in C++, as the user must supply C++ code to define and implement the geometry, to specify the sampling of track information in sensitive detectors, and to instantiate the necessary "manager" objects to initialize and coordinate the simulation. Although C++ skills are part of the culture of high energy particle physics, they are not always as easy to find in other fields, and this has prompted the development of higher-level tools built from Geant4.

Accelerator physicists can benefit from two such tools, BDSIM and G4Beamline. In the following we will describe some of the capabilities of these tools and our development of a prototype model of a TRIUMF beam line in each code. A limitation in BDSIM (being addressed by the code authors at the time of writing) prevented us from advancing to a full simulation, but in G4Beamline we proceeded to refine the model and to validate its tracking and optical properties against measured beam profiles. The validated model enabled us to perform simulations aimed at estimating the influence of multiple scattering in the cyclotron extraction foil on losses in the beam line, of which some first results will be presented.

GEANT4, BDSIM, AND G4BEAMLINE

GEANT4

Geant4 provides a software toolkit for tracking and simulation, in a 3D geometry, of particle interactions in matter. It is object-oriented and scalable to very large and diverse applications. A key characteristic of its design is to allow the user to plug in new or modified simulation components without the need for any modification of the Geant4 code itself.

The code is written in C++ and is implemented as a collection of class libraries in various categories. For a given application, the user provides code for a main program and auxiliary classes which instantiate the components of the simulation: geometry, particles, physics processes, data collection objects (sensitive detectors), and so on. The main program also invokes the "glue", or manager, classes from the toolkit which initialize and coordinate the simulation run. For each instance of an application, the main program and user-written classes are compiled and linked together with the Geant4 libraries to make an executable.

This approach follows the principle that for a simulation code *the most powerful and general input language is the language the code is written in*. For Geant4 any input system less complex than C++ code may limit the expression of complex problems. A somewhat gentler principle is that *a scripting language for object-oriented simulation should itself be object-oriented*.

On the other hand, simpler and easier input methods can be devised for problems with a specialized and well-defined scope, particularly if the scale of the problem is relatively small. For accelerators and beam lines, BDSIM and G4Beamline provide the needed functionality using input methods similar to basic scripting or shell languages.

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BDSIM

BDSIM[2] has been in development since c.2000 and was originally motivated by studies of backgrounds and other issues in the beam delivery systems of next-generation linear colliders (first CLIC and later ILC). The program is conceived in a sufficiently general way to support many other beam line applications. Notably, it incorporates an input parser which allows beam lines defined in MAD(X) language to be rapidly brought into BDSIM with the addition of only a few parameters such as the beam pipe radius and the outer dimensions of magnetic elements.

The other feature that puts BDSIM into a special class of beam simulation programs is that particle tracking in vacuum is done by *element transfer maps*, as in matrix-based codes such as DIMAD and TRANSPORT. The step-wise Geant4 tracking is invoked only when a particle enters a material. Hence, particles that remain in the vacuum chamber are tracked very quickly through the beam line. In studies of beam losses, this allows reduced computation time and improved statistics since the "uninteresting" particles that do not hit anything will be disposed of quickly. This feature also allows easy comparison and benchmarking against other map-based optics and tracking codes.

For the present study, BDSIM presented some limitations that revealed its origin in high-energy collider simulations. Dipole magnets are only of sector bend type (edges perpendicular to the reference path) and edge angles cannot be specified. Although a rectangular bend (RBEND) element is documented, it is in fact implemented as a sector bend. Moreover, the volumes representing dipoles and quadrupoles in the geometry always have circular cross sections. These conditions are not realistic for our application, in which the bends are of rectangular shape, and in which the edge focusing and fringe fields play a significant role in the optics of the beam line.

G4Beamline

G4Beamline[3] has been in development since 2002 and was conceived as a general and flexible interface to Geant4 for studying beam lines. It offers a wide range of beam line components, including the basic magnetic elements as well as rf cavities, solenoids, absorbers and other structures. User-defined elements are also available via a collection of basic Geant4 shapes, with flexible methods for inputting or defining electric and magnetic fields. Each element is described in detail by a set of parameters which can be specified by constants, variable substitution, and general mathematical expressions. For magnets, parameters for gap, field, and iron dimensions, as well as full control over placement and alignment, allow some realism in the geometry and layout of the beam line. A built-in optimization facility allows element parameters to be tuned to specific centering or focusing objectives, or in general to any goal expression in terms of test-particle coordinates.

G4Beamline contains extensive data-collection and processing facilities, including cut-planes, sensitive detector volumes (phantom or inside real elements), powerful event and track cut mechanisms, and beam profile readouts. Data can be output as ascii files, or as Root n-tuples, which can be processed and plotted by the HISTOROOT program supplied with G4Beamline.

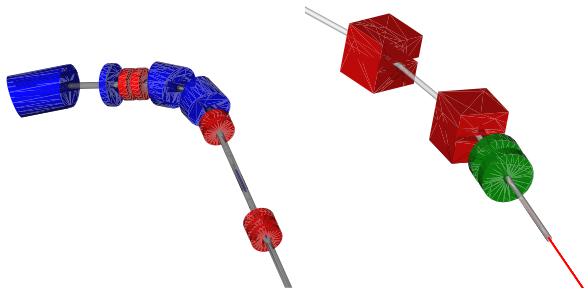

Figure 1: Geant4 visualizations with OpenInventor. The start of BL2A in BDSIM (left) and the end of BL2A in G4Beamline (right) with proton beam emerging

User Experience

Although these programs differ considerably in what is implemented, with G4Beamline generally having a more diverse set of features, the processes of setting up a simulation are quite similar, and the input usually has a 3-part structure: (1) Definition of beams, reference parameters, and other global options; (2) Definition of element prototypes; (3) Layout of the beam line.

Both BDSIM's GMAD input language and the shell-like language used in G4Beamline support element *prototypes* defining common features, as well as element *instances* derived from the prototypes and corresponding to individual elements of the beam line. The instances can have specific names assigned to them, can set additional element parameters, and can override parameters in the prototype. This gives the input an object-oriented structure without the need for formal class definitions.

We also note that both programs can be used interactively with access to Geant4's diverse visualization facilities, which are invaluable for debugging, diagnostic, and informational purposes. The OpenInventor visualization (via Coin3d libraries) in particular offers an efficient and functional interactive 3D viewer for the beam line geometry and particle trajectories, as exemplified in Figure 1.

The two programs differ fundamentally in the way the *reference path* (also called the "reference trajectory" or "design orbit") of the beam line is defined. In BDSIM the reference path is *defined by the sequence of elements*, and is composed of line segments and circular arcs, the latter being defined by the effective lengths and bending angles of the dipole magnets. This makes it extremely easy to lay out the simulated beam line, and follows the convention of many optics and tracking codes. On the other hand, it can be restrictive because in real life some steering dipoles do not involve a bend in the layout of the beam line.

In contrast, in G4Beamline the reference path must be

Figure 2: TRIUMF Beam Line 2A, showing final arc and quadrupole doublet (right) for delivery to ISAC target

explicitly defined by the user as a series of connected line segments. No arcs can be used, and the path through dipoles must be given in a piecewise-linear form, e.g. by bending the path by one-half the bending angle at the entrance and exit of the dipole. Once defined, this path acts as the moving origin for the local coordinate system, in which elements can be positioned and particle trajectories output. This offers greater flexibility and is closer to the way real beam lines are laid out and aligned, but it means that particle coordinates inside dipoles deviate widely from the reference path and are not directly comparable to accelerator coordinates in the conventional curvilinear system.

BEAM LINE 2A

As well as assessing Geant4-based simulation methods, the present study is motivated by their potential application to TRIUMF beam lines, and in particular to Beam Line 2A (BL2A, Figure 2) which supplies 500 MeV protons from the TRIUMF cyclotron to ISOL targets providing rare isotope beams for the ISAC and ISAC II facilities. The reliable performance of BL2A is essential to these multi-user facilities which support experiments in atomic and nuclear physics and nuclear astrophysics.

The beam line, shown schematically in Figure 3 is capable of switching between two independent targets, via the Y-magnet B3, however for present purposes we have modelled only the right-hand branch.

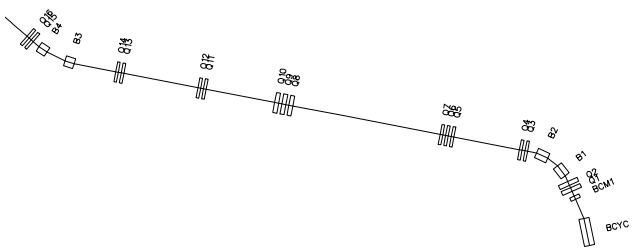

Figure 3: Schematic view of BL2A

BL2A has been providing reliable and stable beam up to 70μA for a number of years, however it has performance issues which motivate further study: (1) It is difficult to tune: doublets and triplets are tightly spaced and focusing is weak in the long straight section; (2) Performance is limited by continuous low-level beam losses, as indicated by beam spill monitors at 38m, 45m and 56m, and by radiation damage on vacuum flange seals at various locations; (3) These losses are not well understood, and it is not known whether tune modifications could reduce the losses.

Extraction to BL2A from the H^- cyclotron is via a 3–5 mg/cm^2 carbon stripping foil at 500MeV radius, converting the H^- to protons which follow exit orbits as shown in Figure 4. This is one of several foils allowing simultaneous extraction to multiple beam lines. The extraction energy can be varied by moving the foil radially and the extracted beam current can be varied by the amount of dipping of the foil vertically into the circulating beam.

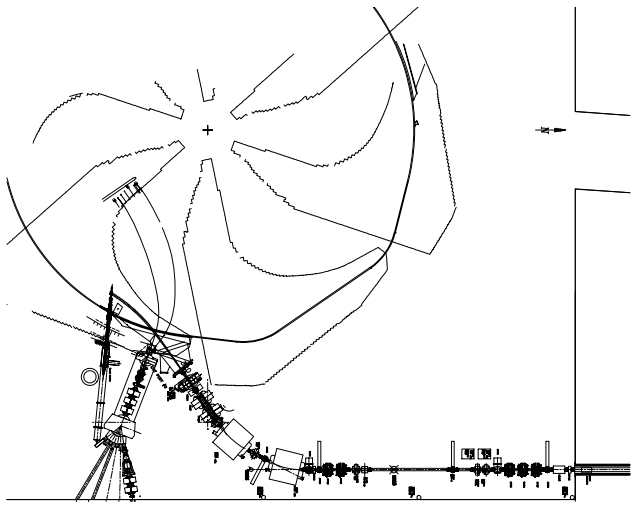

Figure 4: Top view of extraction region for beam line 2A (to the right) and beam line 2C, showing proton orbits.

DEFINING THE STARTING BEAM

Beam characteristics at the extraction foil

The initial conditions of the extracted beam are strong determinates of the beam line optical behaviour and performance. In the extraction process, the location where a circulating H^- ion hits the foil depends on its energy (radius) and on its radial velocity. As shown in Figure 5 this induces a characteristic shape on the extracted beam in horizontal phase space[4] which is not well described by the usual beam ellipse parameters and therefore needs to be input explicitly to G4Beamline. We therefore have used a cyclotron tracking code COMA[5] as a "pre-processor" for G4Beamline to generate up to 10^6 macroparticle coor-

dinates representing the beam distribution at the foil. The COMA coordinates give a good description of the horizontal phase space and the energy distribution of particles. Due to the extreme edge angles of the cyclotron sector magnets, the vertical tracking in COMA is not very accurate. In the following section we describe a different approach used to populate the vertical phase space of the starting beam.

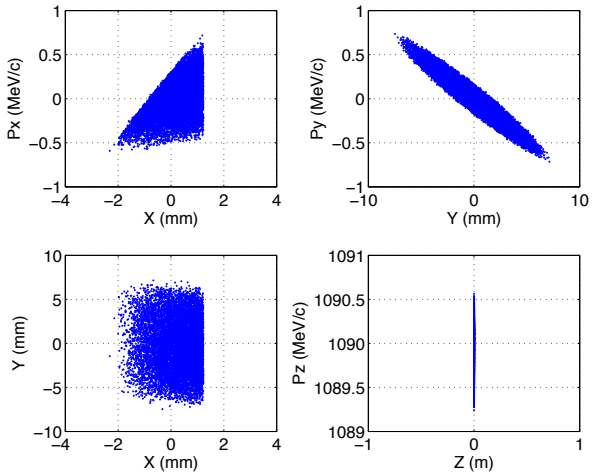

Figure 5: Scatterplot of COMA coordinates at the extraction foil

Optical model

The code TRANSOPTR has been used[6] to develop a model of BL2A which accurately describes the RMS beam characteristics. In this model, the beam sigma matrix parameters at the foil were fitted to beam profile measurements taken from monitors throughout the beam line, using the known dipole and quadrupole settings and estimates of the edge-focusing parameters at the exit from the cyclotron. Although the edge-focusing of the cyclotron magnet is not well quantified in detail, it was found that the aggregate effect could be modelled accurately by using the exit edge-angle of the optical model as an additional free parameter, thus obtaining the improved fit shown in Figure 6 (top).

We used the vertical emittance and ellipse parameters from this model in another simulation code ACCSIM[7] to generate the vertical phase space coordinates for our G4Beamline simulation. The simulation thus has two pre-processors, with the coordinates being merged (consistent with the correct total momentum vector) into an ascii input file which can be sequentially read by G4Beamline.

THE CYCLOTRON FIELD AND EXIT REGION

As seen in the optical model, the edge focusing as the proton beam exits the cyclotron, and in particular the edge angle, are important to the correct behaviour of the model throughout the length of the beam line. Although G4Beamline has an analytical treatment of the fringe fields in dipole magnets (and quadrupoles) it provides only rect-

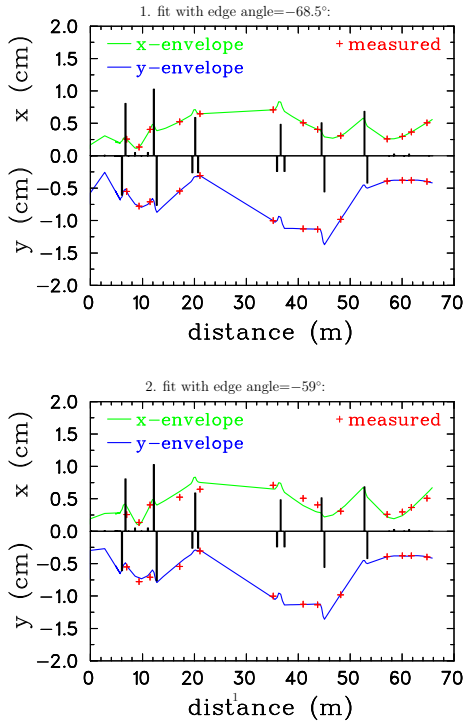

Figure 6: TRANSOPTR envelopes for different (simulated) cyclotron magnet edge angles, compared with measured beam profiles

angular and sector dipole shapes and does not allow an arbitrary edge angle to be specified.

To simulate the −68.5° exit edge angle we used a rectangular bend displaced from the reference path and rotated (Figure 7) so that protons start at the "side" of the magnet and exit at the appropriate angle from the "end" of the magnet, where the fringe field is modelled by G4Beamline.

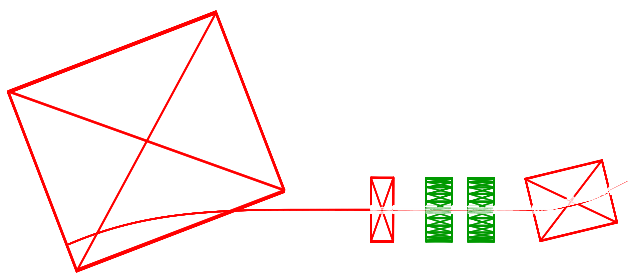

Figure 7: Rotated dipole and central proton trajectory in G4Beamline

Although this scheme gave the correct nominal bending and exit angles, we found that it could not reproduce or even approximate the horizontal focusing and vertical defocusing as seen in the beam envelopes in the optical model and supported by measurements. Although the fringe field depth is an adjustable parameter in G4Beamline we did not find that it was effective, either alone or in conjunction with the dipole edge angle, for tuning the integrated effects of the horizontal and vertical field components to obtain the correct beam envelopes at the cyclotron exit.

This issue will require further study and possibly a dif-

ferent approach to describing the dipole fringe fields. In the meantime we opted to bypass these difficulties by using ACCSIM to track the ensemble from the foil to the cyclotron exit and then export the coordinates to G4Beamline.

VALIDATION WITH ACCSIM + G4BEAMLINE

The simulation code ACCSIM combines matrix tracking with some basic interactions in matter, including Coulomb scattering, energy loss, and nuclear elastic scattering. No secondaries from inelastic interactions are tracked, however virtually all of these from the foil will be outside the acceptance of the beam line and in any case are unlikely to survive the first arc and contribute to downstream losses.

With pre-tracking by ACCSIM, in which a conventional edge-matrix represents the cyclotron edge focusing and fringe field effects, the envelopes of the optical model could be readily and precisely matched using the edge angle as a tuning parameter. Without a foil, the simulation yielded beam envelopes (RMS beam sizes) in good agreement (Figure 8, top) with those of the TRANSOPTR optical model. Introducing the foil in ACCSIM, the resulting envelopes (Figure 8, bottom) agreed very well with measurements, generally within ∼1mm, and in some cases better than the TRANSOPTR envelopes which are derived using an RMS estimate of the emittance growth due to foil scattering.

In view of the sensitivity of the envelopes to initial conditions, and the fact that Geant4 is actually integrating through the dipole and quadrupole fields (with quadrupole strengths identical to those of TRANSOPTR), the close agreement of beam envelopes to the measured ones is remarkable and provides a strong validation of the model construction and of the precision of tracking in Geant4.

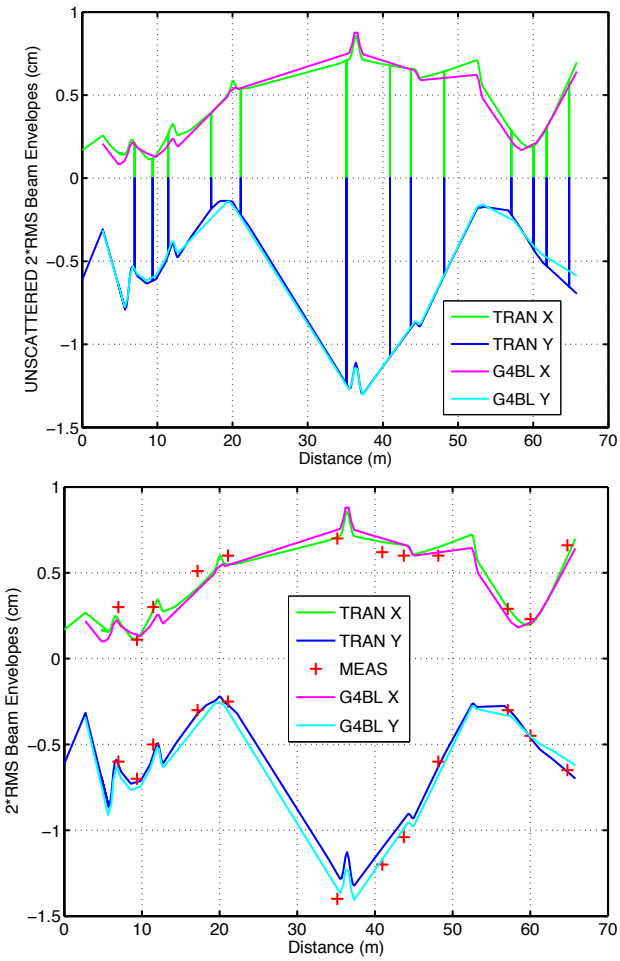

Figure 8: Beam envelopes from TRANSOPTR and G4Beamline compared for unscattered beam (top) and compared with measurements for scattered beam (bottom)

LOSSES DUE TO THE CYCLOTRON EXTRACTION FOIL

In a 5 mg/cm^2 extraction foil, Coulomb scattering is by far the dominant process contributing to the initial loss of protons in the cyclotron exit region and the first arc of BL2A. There are much smaller contributions from nuclear interactions, at about the 10^{-5} level, and from the very long but very sparsely populated Landau tail of the ionization energy loss distribution.

Most protons scattered to angles of more than a few milliradians will be lost within the cyclotron tank itself or in the exit horn region. Of the remainder initially accepted into BL2A, most will be lost in the first arc. A long-standing question is whether foil scattering plays any role in the distributed low level losses downstream. Initially we observed no losses at all when we introduced the extraction foil, either in a full G4Beamline simulation (with exaggerated envelopes due to the aforementioned cyclotron field problems) or in the ACCSIM-pre-tracked simulation. In both cases, multiple-scattering models are used which are not at their best in such thin layers of material.

Scrutinizing the multiple scattering in ACCSIM, which is based on Molière theory with subsequent corrections and refinements, we observed that for this foil the unprojected scattering angle cuts off at around 3 milliradians, whereas the angular acceptance of the beam line with respect to the foil is roughly 10mr. Neither model includes the H^- stripping, but the preliminary analysis of the foil in ACCSIM indicated that protons traversing the entire foil thickness would undergo an average of only ∼125 scatters.

Fortunately ACCSIM also has an iterated-single-scatter model for use in very thin foils. This model revealed the shortcomings of the multiple scattering treatment: for statistics of 10^6 protons a fraction of 4.2×10^{-4} of the beam was scattered into angles >3mr and extending out to ∼100mr. This fraction is significant for a 70μA beam, since previous experiments with BL2A[8] established that mis-steering as little as 1 nA of beam at the first dipole resulted in measurable losses at the downstream spill monitors.

Accordingly we "forced" the single-scatter model in ACCSIM and used it to generate a "halo beam" consisting only of protons scattered beyond 3mr (Figure 9). This

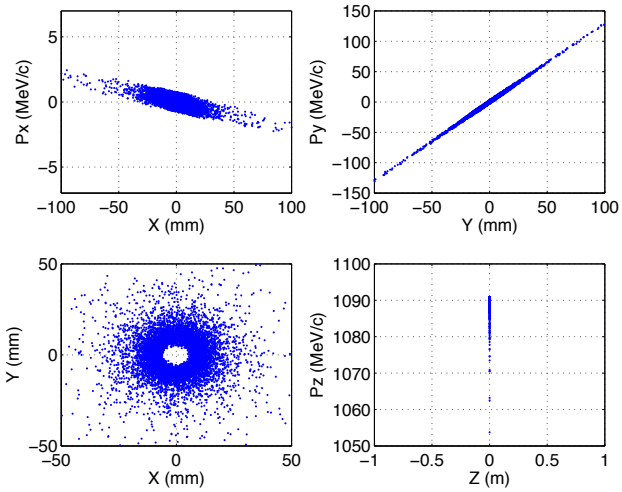

Figure 9: ACCSIM-generated halo beam around 3mr cone

ensemble was pre-tracked in ACCSIM to the cyclotron exit and then tracked in G4Beamline. Geant4 by default tracks all secondaries from the proton interactions, so we invoked G4Beamline's `kill=1` option on all the beam line components. This option stops protons as soon as they hit anything, and thus indicates the location of primary particle losses.

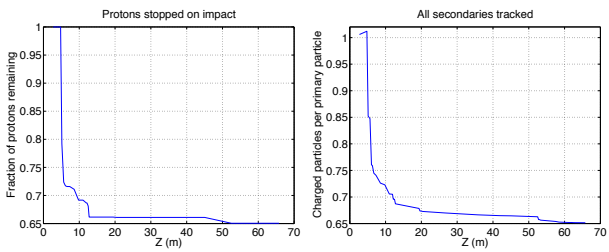

Figure 10: Left: survival of 3mr halo primary protons (all protons stopped on impact). Right: survival of charged particles (all secondaries tracked). Note lower axis limits.

As shown in Figure 10, about 65% of the halo beam is transmitted by the beam line. Of the remainder, almost all is lost within 12m, comprising the first arc and following quadrupole doublet. However, about 1% of the halo survives until ∼45m where it is lost in the next 7m (Q13/14 region). This region is of interest due to somewhat elevated routine spill monitor readings and radiation damage observed on a flange seal near the final arc.

In a subsequent run all secondaries were tracked and the resulting flux of charged particles (in principle detectable by spill monitors) is shown in Figure 10. Although detectable losses do propagate downstream, there is the indication of a "shadow" due to Q14 at 53m which may limit the diagnostic capacity of spill monitor BSM32 at 56m.

These results represent the rather ideal situation of a nearly perfectly-centered (within 0.5mm) beam line with perfectly-aligned elements free of field errors. In geometrical terms at least, this is the first tangible evidence that extraction foil scattering may contribute to losses far downstream from the foil location.

CONCLUSIONS AND ACKNOWLEDGMENTS

Using input methods similar to those of optics and tracking codes, BDSIM and G4Beamline fulfill the promise of being able to develop a full-fledged Geant4 simulation of a beam line without any need for C++ programming and with much less effort. Although BDSIM was not completely adaptable to our application, we expect that it will continue to be developed and generalized, as it occupies a unique position with its combination of fast transfer maps in vacuum with Geant4 tracking in materials.

In G4Beamline we were able to proceed to an accurate model which was validated against measured beam envelopes. Using an iterated single-scatter treatment of Coulomb scattering in the cyclotron extraction foil, we established a baseline loss rate due to foil scattering of $\sim$1.4x10^{-5} of the total beam intensity for a 5mg/cm^2 foil. The G4Beamline model will be used to explore other possible loss mechanisms, such as field and alignment errors, as well as to study possible improvements in loss control, detection and monitoring.

These programs are significant achievements in the quest for realistic and predictive simulations of beam lines. We would like to thank the authors of BDSIM (Graham Blair, Ilya Agapov, Steve Malton, Lawrence Deacon) and the author of G4Beamline (Tom Roberts) for sharing their work and for answering many email queries as well as providing indispensable guidance and advice.

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