

An Algorithm for Computing Screened Coulomb Scattering in GEANT4¹

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Abstract

An algorithm has been developed for the GEANT4 Monte-Carlo package for the efficient computation of screened Coulomb interatomic scattering. It explicitly integrates the classical equations of motion for scattering events, resulting in precise tracking of both the projectile and the recoil target nucleus. The algorithm permits the user to plug in an arbitrary screening function, such as Lens-Jensen screening, which is good for backscattering calculations, or Ziegler-Biersack-Littmark screening, which is good for nuclear straggling and implantation problems. This will allow many of the applications of the TRIM and SRIM codes to be extended into the much more general GEANT4 framework where nuclear and other effects can be included.

Key words:

Geant4, Screened Scattering, Coulomb Scattering, Elastic Recoil, Nuclear Stopping Power, NIEL, Non-Ionizing Energy Loss, TRIM, SRIM, Displacement Damage
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1 Introduction

The necessity of accurately computing the characteristics of interatomic scattering arises in many disciplines in which energetic ions pass through materials. Traditionally, solutions to this problem not involving hadronic interactions have been dominated by the well-known TRIM [1] and SRIM [2,3] codes. These codes take a Monte-Carlo approach to computing distributions of ions passing through a material, and use a universal parameterized formula to determining a scattering angle for a particle which collides with a target nucleus. This formula is a parameterization of the scattering integrals computed from a parameterization of an interatomic screening function. This approach is reasonably successful, but not very flexible. In particular, it is relatively difficult to introduce into such a system a particular screening function which has been measured for a specific atomic pair, rather than the universal functions which are applied.

In recent years, a more general framework, GEANT4 [4,5], is being developed by the high-energy physics community for the handling of the motion of energetic particles through matter. Like TRIM and SRIM, it takes a Monte-Carlo approach to produce statistical distributions of particles as they move through various types of matter. However, the GEANT4 collaboration has developed a much larger toolkit than SRIM for handling very complex geometries, and for including many physical processes other than just the traditional electronic stopping and nuclear stopping in its computation. In many problems of current interest, such as the behavior of semiconductor device physics in a space environment, nuclear reactions, particle showers, and other effects are critically important in modeling the full system. Thus, it is important to have components in the GEANT4 toolkit to bridge the gap between the effective handling of low-energy processes in simple geometries provided by SRIM and the very general framework for nuclear events and complex geometries already available in GEANT4.

To be consistent with the general GEANT4 philosophy of providing tools which are flexible and extensible as better physics models become available, it was decided that introducing Ziegler-Biersack-Littmark (ZBL) universal scattering method [6] into GEANT4 was inappropriately limiting. Although for most problems to which SRIM is applied, the accuracy of the universal scattering equations is sufficient, it is easy to imagine that for situations in which precise event rates are needed, one might wish to include high-precision measured interatomic potentials into a computation. The approach described below makes this very simple, while allowing one to use the well-established ZBL screening function [7] (but not the ZBL 'magic formula' for scattering integrals) for the many situations in which it is sufficiently accurate.

2 Method

The method used in this computation is a variant of a subset of the method described by the authors in a previous paper [8]. A very short recap of the basic material is included here. The scattering of two atoms from each other is assumed to be a completely classical process, subject to an interatomic potential described by a potential function

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \phi\left(\frac{r}{a}\right) \quad (1)$$

where Z_1 and Z_2 are the nuclear proton numbers, e^2 is the electromagnetic coupling constant ($q_e^2/4\pi\epsilon_0$ in SI units), r is the inter-nuclear separation, ϕ is the screening function describing the effect of electronic screening of the bare nuclear charges, and a is a characteristic length scale for this screening. In most cases, ϕ is a universal function used for all ion pairs, and the value of a is an appropriately adjusted length to give reasonably accurate scattering behavior. In the method described here, there is no particular need for a universal function ϕ , since the method is capable of directly solving the problem for most physically plausible screening functions. It is still useful to define a typical screening length a in the calculation described below, to keep the equations in a form directly comparable with our previous work even though, in the end, the actual value is irrelevant as long as the final function $\phi(r)$ is correct. From this potential $V(r)$ one can then compute the classical scattering angle from the reduced center-of-mass energy $\varepsilon \equiv E_c a / Z_1 Z_2 e^2$ (where E_c is the kinetic energy in the center-of-mass frame) and reduced impact parameter $\beta \equiv b/a$

$$\theta_c = \pi - 2\beta \int_{x_0}^{\infty} f(z) dz/z^2 \quad (2)$$

where

$$f(z) = \left(1 - \frac{\phi(z)}{z\varepsilon} - \frac{\beta^2}{z^2}\right)^{-1/2} \quad (3)$$

and x_0 is the reduced classical turning radius for the given ε and β .

The problem, then, is reduced to the efficient computation of this scattering integral. In our previous work, a great deal of analytical effort was included to proceed from the scattering integral to a full differential cross section calculation, but for application in a Monte-Carlo code, the scattering integral $\theta_c(Z_1, Z_2, E_c, b)$ and an estimated total cross section $\sigma_0(Z_1, Z_2, E_c)$ are all that is needed. Thus, we can

skip algorithmically forward in the original paper to equations 15-18 and the surrounding discussion to compute the reduced distance of closest approach x_0 . This computation follows that in the previous work exactly, and will not be reintroduced here.

For the sake of ultimate accuracy in this algorithm, and due to the relatively low computational cost of so doing, we compute the actual scattering integral (as described in equations 19-21 of [8]) using a Lobatto quadrature of order 6, instead of the 4th order method previously described. This results in the integration accuracy exceeding that of any available interatomic potentials in the range of energies above those at which molecular structure effects dominate, and should allow for future improvements in that area. The integral α then becomes (following the notation of the previous paper)

$$\alpha \approx \frac{1 + \lambda_0}{30} + \sum_{i=1}^4 w'_i f\left(\frac{x_0}{q_i}\right) \quad (4)$$

where

$$\lambda_0 = \left(\frac{1}{2} + \frac{\beta^2}{2x_0^2} - \frac{\phi'(x_0)}{2\varepsilon} \right)^{-1/2} \quad (5)$$

and

$$w'_i \in [0.03472124, 0.1476903, 0.23485003, 0.1860249]$$

and

$$q_i \in [0.9830235, 0.8465224, 0.5323531, 0.18347974]$$

(See appendix A). Then

$$\theta_c = \pi - \frac{\pi\beta\alpha}{x_0} \quad (6)$$

The other quantity required to implement a scattering process in GEANT4 is the total scattering cross section σ_0 for a given incident ion and a material through which the ion is propagating. This value requires special consideration for a process such as screened scattering. In the limiting case that the screening function is unity, which corresponds to Rutherford scattering, the total cross section is infinite. For various screening functions, the total cross section may or may not be finite. However, one must ask what the intent of defining a total cross section is, and determine from that how to define it.

In GEANT4, the total cross section is used to determine a mean-free-path l_μ which is used in turn to generate random transport distances between discrete scattering

events for a particle. In reality, where an ion is propagating through, for example, a solid material, scattering is not a discrete process but is continuous. However, it is a useful, and highly accurate, simplification to reduce such scattering to a series of discrete events, by defining some minimum energy transfer of interest, and setting the mean free path to be the path over which statistically one such minimal transfer has occurred. This approach is identical to the approach developed for the original TRIM code [1]. As long as the minimal interesting energy transfer is set small enough that the cumulative effect of all transfers smaller than that is negligible, the approximation is valid. As long as the impact parameter selection is adjusted to be consistent with the selected value of l_μ , the physical result isn't particularly sensitive to the value chosen. One of the sets of validation tests discussed below will verify the truth of this hypothesis, and will determine what reasonable values for this minimal energy transfer are.

Noting, then, that the actual physical result isn't very sensitive to the selection of l_μ , one can be relatively free about defining the cross section σ_0 from which l_μ is computed. The choice used for this implementation is fairly simple. Define a physical cutoff energy E_{min} which is the smallest energy transfer to be included in the calculation. Then, for a given incident particle with atomic number Z_1 , mass m_1 , and lab energy E_{inc} , and a target atom with atomic number Z_2 and mass m_2 , compute the scattering angle θ_c which will transfer this much energy to the target from the solution of

$$E_{min} = E_{inc} \frac{4 m_1 m_2}{(m_1 + m_2)^2} \sin^2 \frac{\theta_c}{2} \quad (7)$$

and then solve, by iterative inversion of eq. (6), the value of the impact parameter b at which this value of θ_c is achieved. Then, define the total cross section to be $\sigma_0 = \pi b^2$, the area of the disk inside of which the passage of an ion will cause at least the minimum interesting energy transfer. Because this process is relatively expensive, and the result is needed extremely frequently, the values of $\sigma_0(E_{inc})$ are precomputed for each pairing of incident ion and target atom, and the results cached. However, since the actual result isn't very critical, the cached results can be stored in a very coarsely sampled table without degrading the calculation at all, as long as the values of the l_μ used in the impact parameter selection are rigorously consistent with this table.

The final necessary piece of the scattering integral calculation is the statistical selection of the impact parameter b to be used in each scattering event. This selection is done following the original algorithm from TRIM, where the cumulative probability distribution for impact parameters is

$$P(b) = 1 - \exp\left(\frac{-\pi b^2}{\sigma_0}\right) \quad (8)$$

where $N \sigma_0 \equiv 1/l_\mu$ where N is the total number density of scattering centers in the target material and l_μ is the mean free path computed in the conventional way. To produce this distribution from a uniform random variate r on $(0,1]$, the necessary function is

$$b = \sqrt{\frac{-\log r}{\pi N l_\mu}} \quad (9)$$

This choice of sampling function does have the one peculiarity that it can produce values of the impact parameter which are larger than the impact parameter which results in the cutoff energy transfer, as discussed above in the section on the total cross section, with probability $1/e$. When this occurs, the scattering event is not processed further, since the energy transfer is below threshold. For this reason, impact parameter selection is carried out very early in the algorithm, so the effort spent on uninteresting events is minimized.

The above choice of impact sampling is modified when the mean-free-path is very short. If $\sigma_0 > \pi \left(\frac{l}{2}\right)^2$ where l is the approximate lattice constant of the material, as defined by $l = N^{-1/3}$, the sampling is replaced by uniform sampling on a disk of radius $l/2$, so that

$$b = \frac{l}{2} \sqrt{r} \quad (10)$$

This takes into account that impact parameters larger than half the lattice spacing do not occur, since then one is closer to the adjacent atom. This also derives from TRIM.

One extra feature is included in our model, to accelerate the production of relatively rare events such as high-angle scattering. This feature is a cross-section scaling algorithm, which allows the user access to an unphysical control of the algorithm which arbitrarily scales the cross-sections for a selected fraction of interactions. This is implemented as a two-parameter adjustment to the central algorithm. The first parameter is a selection frequency f_h which sets what fraction of the interactions will be modified. The second parameter is the scaling factor for the cross-section. This is implemented by, for a fraction f_h of interactions, scaling the impact parameter by $b' = b/\sqrt{scale}$. This feature, if used with care so that it does not provide excess multiple-scattering, can provide between 10 and 100-fold improvements to event rates. If used without checking the validity by comparing to un-adjusted scattering computations, it can also provide utter nonsense. This scaling provides a mechanism to address the issues discussed in the recent literature [9,10]. In particular, it solves the problem of preserving multiple scattering effects by leaving most interactions unaffected (if the fraction f_h is much less than unity) while still providing significantly enhanced yields of hard collisions.

3 Validation

There are a number of features of this model which need to be verified against good physical data and theoretical expectations, within the GEANT4 framework, to assure the compatibility of its statistical sampling methods with those of GEANT4, the correctness of the underlying physical assumptions, and the freedom of the implemented code from logic defects.

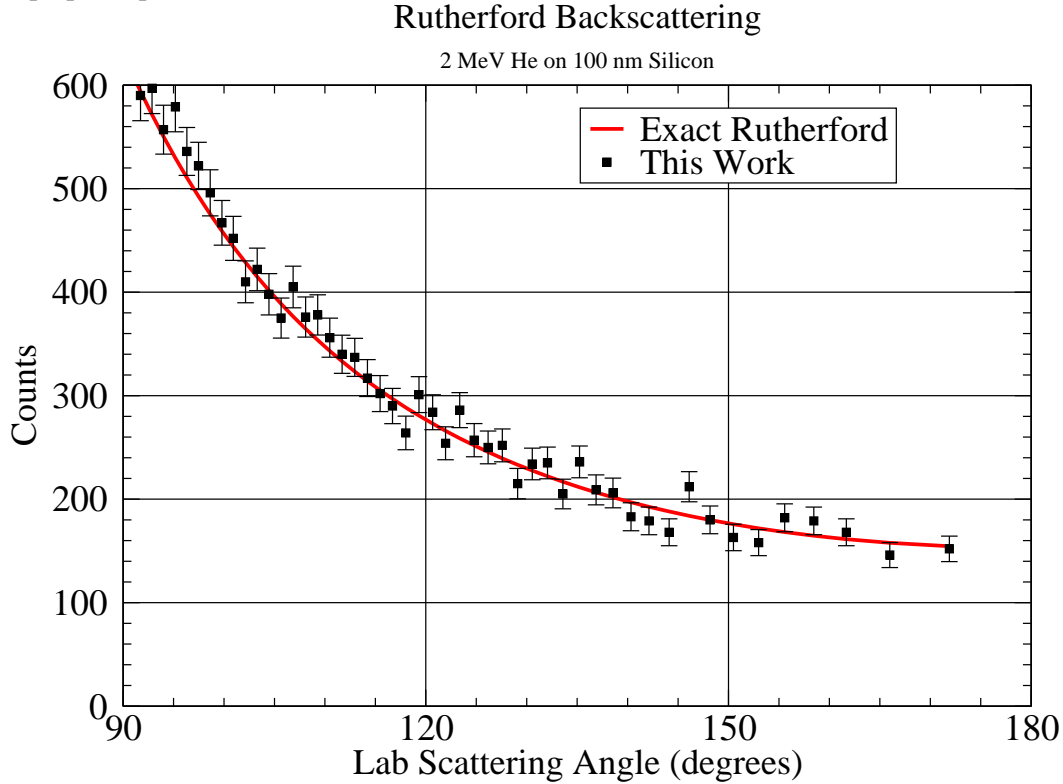
In many of the comparisons below, we use data from SRIM as the reference. This choice was made because of the wide acceptance of SRIM in many fields as a useful and well-tested tool. Furthermore, the large compendium of measurements referenced at [3] provides a central repository for such information. However, precise agreement with SRIM is not the goal of these comparisons. The method we describe should be more accurate than the nuclear scattering component of SRIM, in that it exactly integrates the scattering, rather than using a universal, parameterized approximation to it. Further, this method can be applied with specific internuclear potentials, allowing further enhancement in accuracy over SRIM. However, since electronic stopping contributes to all the processes discussed below, and SRIM is highly optimized for this, especially in compound materials, it will most likely provide different, and probably better, results in some domains.

In the results below, the smooth curves listed as SRIM data are digitized from the curves on the graphs provided on the SRIM website as of May, 2004. The digitized data was oversampled, and then smoothed via least-squares cubic splining. If a reader of this work intends to digitize data from our graphs, it is highly recommended that the SRIM data be obtained from the original, and not re-digitized from our copy, to prevent accumulation of errors.

Rutherford Scattering

The first, and most basic, test is to see if the code replicates well-known scattering distributions. It is important to note that, for this method, the Rutherford cross-section is not a special case, insofar as the integrand in eq.(2) does not reduce to an unusually simple form under our selected change-of-variable. Thus, agreement with the expectations of Rutherford scattering, under conditions where this cross-section is accurate, is a strong test of validity. To make this comparison, a very typical set of scattering parameters was chosen, which is the scattering of 2 MeV α particles from a 100 nm thick silicon foil. The results shown in Figure 1 were computed both for the unmodified cross-section, and for a cross-section increased

Fig. 1. This compares the backscattering of 2 MeV α particles from a 100 nm Si foil to the theoretical value. A total of 10^8 particles were used, with a cross-section enhancement of 100, to get these statistics. The data are binned in $\cos \theta$ bins with $\Delta \cos \theta = 0.02$. The points are plotted at the bin center, transformed to an angle. Computing time on a modern laptop computer is a few hours.

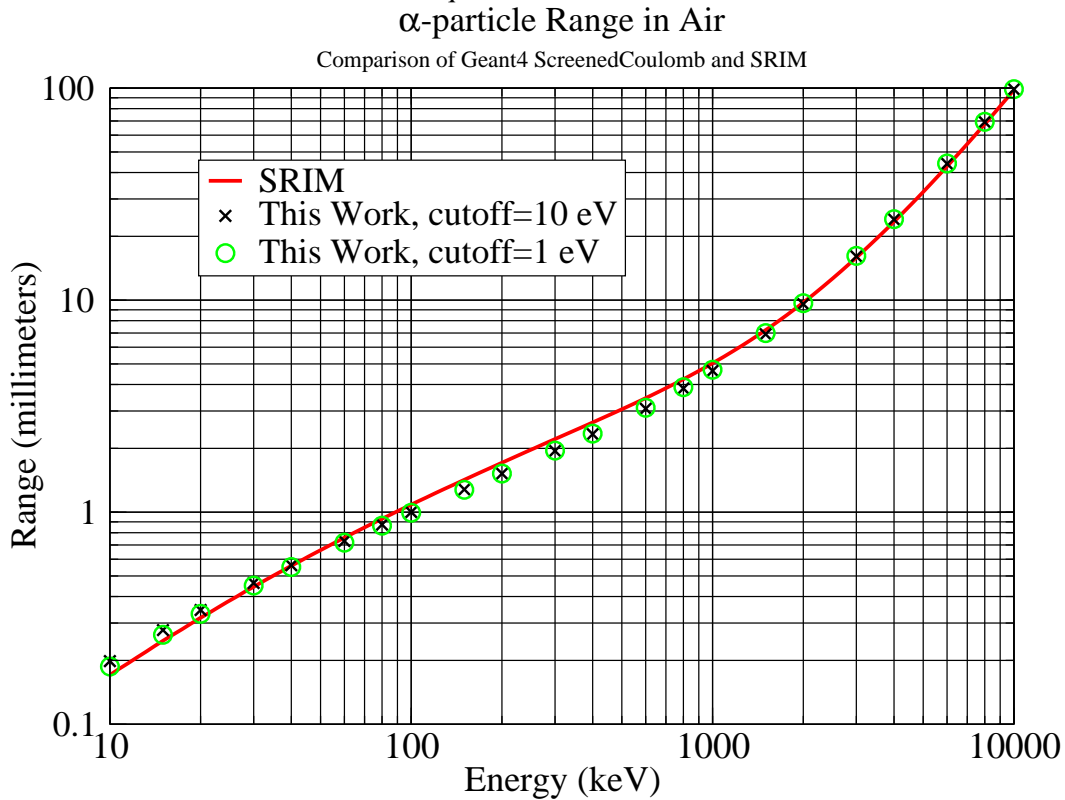


by a factor of 100, as described above. The excellent agreement between the two results indicates that the scaling process is not distorting the calculation. The scaled cross section is used in the final statistical comparison, since the total number of events is much larger, resulting in better statistics. In the case of this calculation, where the scattering probability from such a thin target is very small for almost all scattering angles greater than 10 degrees, and multiple scattering provides no significant contribution, this agreement, even with a large cross-section scaling, is expected. Note that the calculation has been cut off for small scattering angles, where deviations from the Rutherford cross-section arise and where this assumption about multiple scattering is not valid. Other validation tests will cover this region.

Ion Implantation and Range Straggling

To test the process described here for accuracy in final stopping situations, we will compare with two very well documented systems: the propagation of α particles in air, shown in figure 2, which has been studied since 1913 (see, *e.g.*, [11] and an extensive bibliography at [3]), and the implantation of dopants in silicon, which has

Fig. 2. Alpha particle range in air. Even at the lowest energies for which data are available, this process is dominated by electronic stopping. Thus, the differences which errors in our calculation would introduce here are quite small.



been thoroughly studied because of its importance to the semiconductor industry. The two cases for implantation also cover two very different regions of parameter space. The implantation of boron in silicon involves a light projectile on a heavy target, where some high-angle scattering events can occur. Conversely, for arsenic in silicon, where the projectile is much heavier than the target, all scattering is very forward. Also, the arsenic-in-silicon test case samples data down to extremely low velocity. These are shown in figures 3 and 4.

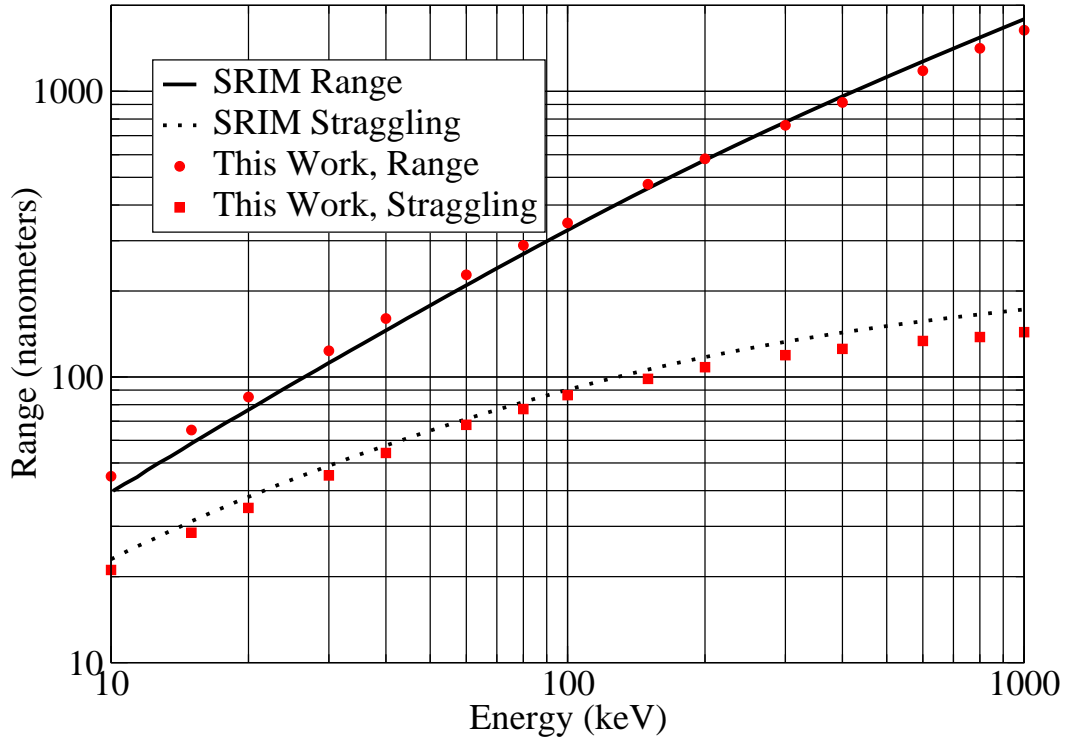
Forward Multiple Scattering

The ability of this process to correctly produce small-angle forward scattering is likely to be quite important. Typically, one is interested in the diffusion of an incoming beam particle as it is transported through, for example, a gas cell or metal vacuum window. Although GEANT4 includes its own multiple scattering process to approximate this, that process is optimized for efficiency with very high energy

Fig. 3. Boron range and straggling in silicon. At high energies, where most of the energy loss is electronic, straggling is small and the implantation profile is very narrow.

Boron Implantation in Silicon

Geant4 ScreenedCoulomb comparison to SRIM

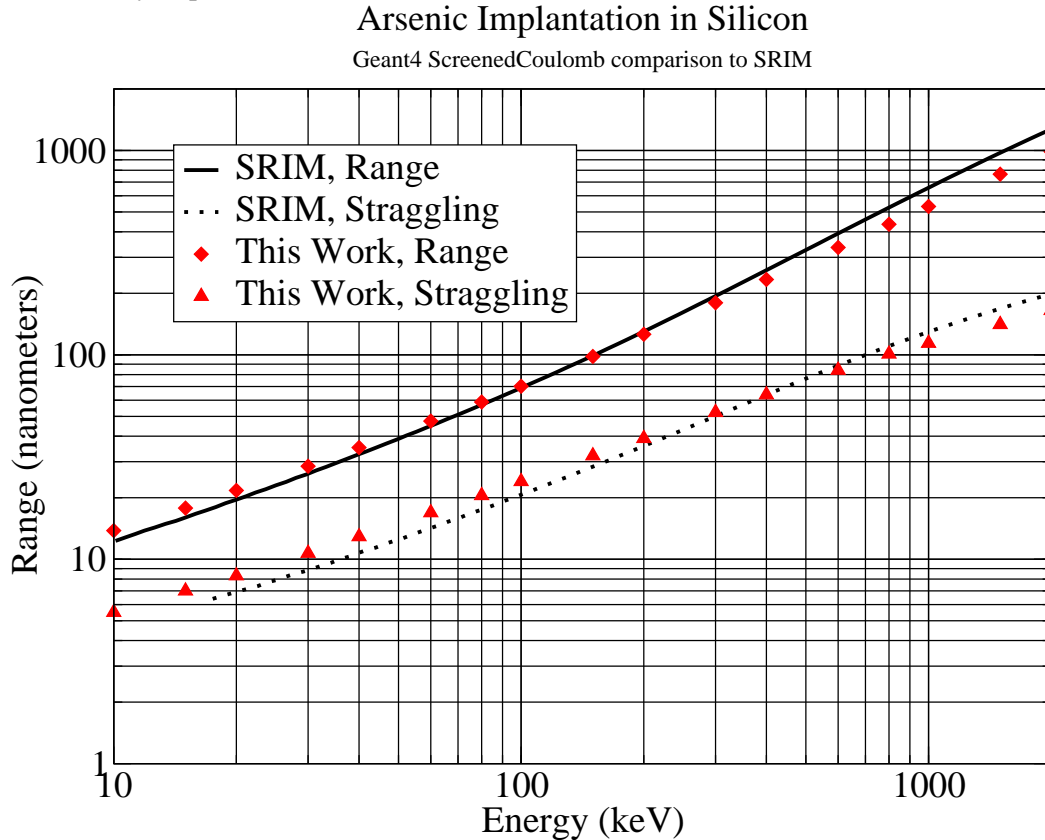


ions, and for cases in which such scattering is quite weak.

Since the authors of this work have previous experience with and interest in scattering of 270 keV α particles for surface analysis, we chose a test case from this domain. The data presented in Figure 5 show the results. On two of the curves, representative raw data from the Monte-Carlo simulation are shown, to illustrate typical counting statistics for the data from which these curves are computed. The actual smooth curves are least-squares cubic splines of the data.

The effect of the low-energy cutoff of this process is apparent at very small angles, where scattering is suppressed below about 0.02 radians. This should be considered as a warning to users of this process, in that one must consider carefully what scattering angles are of interest. Choosing the cutoff energy too high will result in distortion of the scattering distribution for small angles, but can result in improved computational speed. In the case of this foil, the mean-free-path is about 30% of the foil thickness for the 10 eV cutoff, and about 5% of the foil thickness for the 1 eV cutoff. It is likely that this is a good way to estimate an appropriate cutoff energy, since good multiple scattering accuracy depends upon at least a few interactions being applied to each ion passing through the target. With the cutoff at 10 eV, for

Fig. 4. Arsenic range and straggling in silicon. At the relatively low velocities associated with the kinetic energy range covered by this data set, nuclear scattering is strong, so the straggling is a large fraction of the projected range and the process described in this work is extremely important.



this foil thickness, one is primarily sampling ions which have not undergone many scatterings in the foil, so the distribution is somewhat too narrow. By the time the cutoff has been reduced to 1 eV, each ion is scattered about 20 times in the foil, and the resulting statistics can be expected to be quite accurate.

The curve labeled 'Quasi-analytic' is computed using the method of [12], adapted for the case where the energy of the beam exiting the target is very different from the initial energy. This technique is a small-angle approximation to the multiple scattering, but it uses high-accuracy scattering cross-sections computed directly from the screening functions.

The curve labeled 'Geant4 MSC' uses the G4MultipleScattering (MSC) process which is a standard part of the GEANT4 package. This process uses a statistical approach to multiple scattering [13], somewhat similar to that of [12], but which is based on universal, parameterized scattering cross sections. As can be seen from the graph, it severely underestimates high-angle scattering for heavy ions. More significant, and one of the primary reasons for this work, is that it does not produce recoil particles.

Fig. 5. Forward scattering of 270 keV α particles from a $100 \mu\text{g}/\text{cm}^2$ carbon foil.

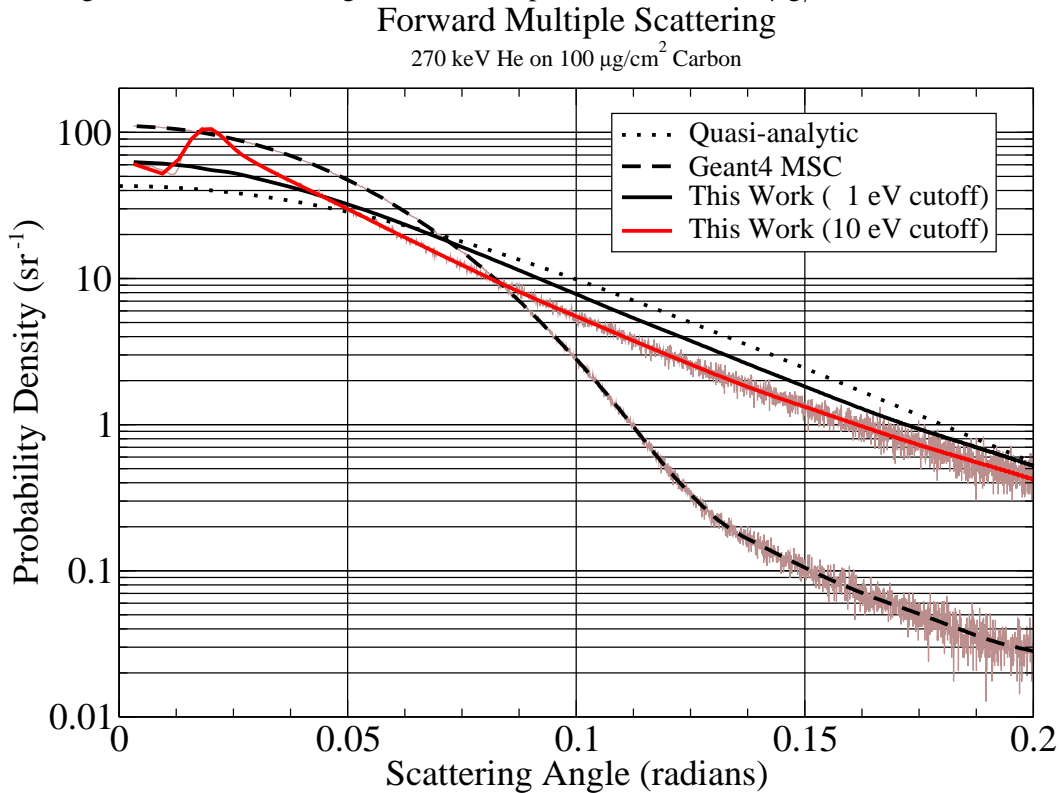
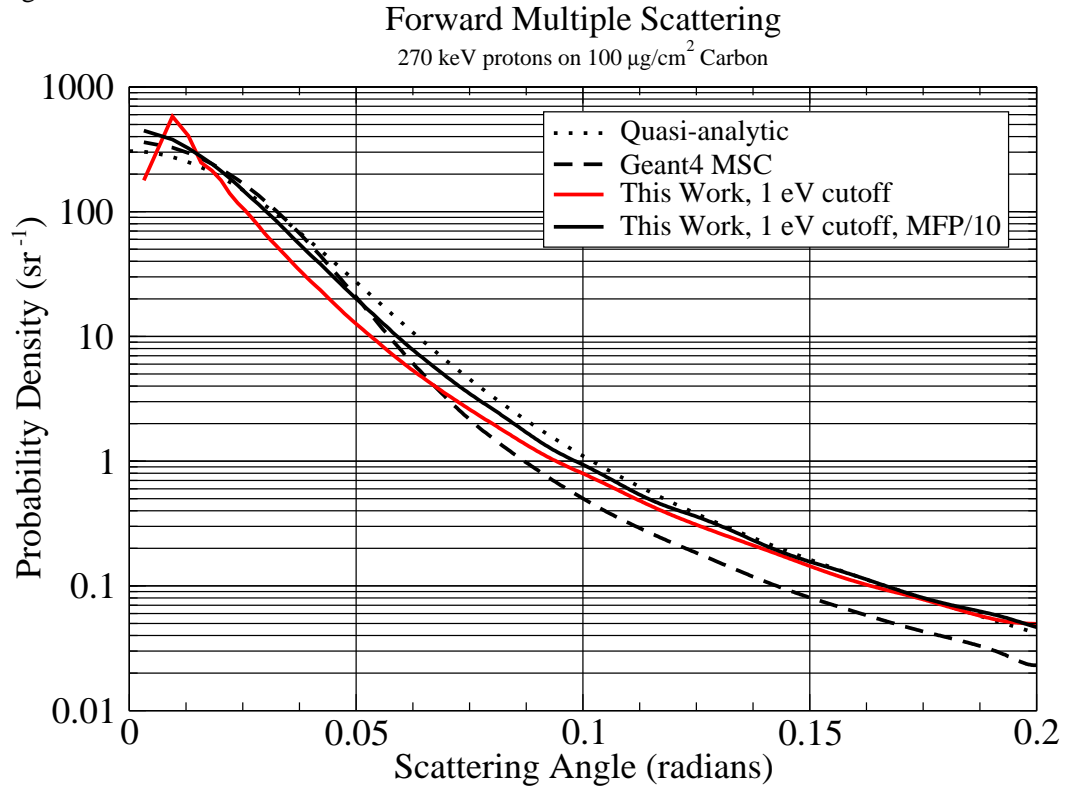


Figure 6 shows another forward multiple-scattering case, with two important differences from that in Figure 5. First, the intrinsic GEANT4 multiple scattering works quite well for computing the width of the forward scattering distribution for protons. Note that, even for this case, it shows a deficit of almost a factor of two for higher-angle scattering. Second, another parameter of the the screened Coulomb model is exercised in this run.

In the discussion above, the mean free path was adjusted to be substantially less than the target thickness by adjusting the lower cutoff energy of the data tables being built. In the case of protons at this energy, even with a 1 eV cutoff energy, the mean free path is too long to get good results. Lowering the physics cutoff below 1 eV is probably unphysical, since the potentials aren't well known far into the tails, and solid state effects probably make them meaningless. However, the real problem with the long mean free path is not that any physics is missing; it is that many particles get through with zero scattering events, since the mean number of events is only a few.

The model contains a parameter `MFPScale` which allows the user to artificially shorten the mean free path in a consistent manner, so that more attempts are made to scatter and the Poisson statistics don't overlap zero events very strongly. This allows the user to adjust the model for the case of very thin foils. The curve labeled 'MFP/10' has had the mean free path reduced a factor of 10, and this fully resolves

Fig. 6. Forward scattering of 270 keV protons from a $100 \mu\text{g}/\text{cm}^2$ carbon foil. In this case, agreement between MSC and this work is close.



(at the expense of increased computing time) the shape of the scattering distribution near the origin.

4 Conclusions

The algorithm presented here provides an accurate and efficient way to include the effects of Coulomb scattering and the generation of recoil particles in GEANT4 simulations. This algorithm has the flexibility to permit the user to select screening functions appropriate for specific applications, and to provide new screening functions, without any rewriting of the core code. It should find wide applicability in many problems in the interaction of fast ions with materials, where the average multiple-scattering already provided by GEANT4 must be replaced by a detailed model.

Some improvements may be possible in the future, with appropriate checks for physical validity. It is the belief of the authors that the weighting of the target atom selection could be improved with extra material information. In a material in which atoms live in very different environments, weighting the selection by the mean-square bond length for each specific species may improve the statistical selection

accuracy. This would provide some compensation for an atom being closely caged by its neighbors, such that it is hard to hit that atom without also making a close pass to other species. Such weighting would have to be implemented by providing extra information for the target material, beyond that which GEANT4 normally uses. A mechanism for this already exists in GEANT4.

Although the current implementation of the algorithm is strictly non-relativistic, the authors are investigating simple extensions which will correctly handle small-angle collisions for relativistic incident particles and non-relativistic recoils. These collisions are important for nuclear stopping power and Non-Ionizing Energy Loss (NIEL) calculations at high energies. Hard collisions at relativistic energies are not to be included, since such collisions have a small Coulombic cross-section and will be combined hadronic-Coulombic events, in which case the screening function and classical scattering concepts are not valid, and the resulting processes are handled by nuclear-reaction codes.

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A Appendix: Derivation of Integration Constants

The coefficients for the summation to approximate the integral for α in eq.(4) are derived from the values in Abramowitz & Stegun [14, sec. 25.4.32 and table 25.6], altered to make the change-of-variable used for this integral. There are two basic steps to the transformation. First, since the provided abscissas x_i and weights w_i are for integration on $[-1,1]$, with only one half of the values provided, and in this work the integration is being carried out on $[0,1]$, the abscissas are transformed as:

$$y_i \in \left\{ \frac{1 \mp x_i}{2} \right\} \quad (\text{A.1})$$

Then, the primary change-of-variable is applied resulting in:

$$q_i = \cos \frac{\pi y_i}{2} \quad (\text{A.2})$$

$$w'_i = \frac{w_i}{2} \sin \frac{\pi y_i}{2} \quad (\text{A.3})$$

except for the first coefficient w'_1 where the $\sin()$ part of the weight is taken into the limit of λ_0 as described in eq.(5). This value is just $w'_1 = w_1/2$.

B Appendix: GEANT4 Implementation

The process being described in this work is a process of class `G4DiscreteProcess` in the GEANT4 class hierarchy. As such, it really only needs to provide a few functions to interact correctly with the GEANT4 world. The functions used by GEANT4 are the constructor, `GetMeanFreePath()`, and `PostStepDoIt()`. Internally, the functions are divided into two classes, a private `CrossSection` class which handles loading of screening tables and total cross-section tables, and the main `ScreenedNuclear-Recoil` class, which implements the required `G4DiscreteProcess` interface. There are a few other utilities provided which allow such functions as adjusting various model cutoffs, cross-section biasing, and control of energy deposition. The computation and caching of screening functions and total cross-sections is left to an external PYTHON [15] program.

Class CrossSection

This is a class derived from `G4CrossSectionHandler`, and provides extensions to that class to read data in via a pipe from an external process, and to store screening tables along with cross section tables.

Method: LoadData(G4String screeningKey, G4int z1, G4double m1, G4double recoilCutoff)

This method is the primary reason for the existence of this class. The standard `G4CrossSectionHandler` class is designed to read precomputed cross sections from stored text files in a fixed format. For the purposes of this system, it is not only necessary to have cross sections, but screening tables, and these tables depend on the value of the minimum scattering energy cutoff, as described above. The number of available parameters would result in a combinatorially large number of files being required in the database. To avoid this problem, the author decided that it was more efficient to use a small, external program, written in the PYTHON programming language, to dynamically generate the files as needed and to maintain a cache of the tables actually used for quick re-use. This permits the user to include custom screening functions by adding them to a small, easily maintained PYTHON module. This module returns data to the main program through a UNIX-style pipe interface, which is supported on all POSIX-compatible platforms, and appears as a file to both the calling and called program.

Method: SelectRandomTargetUnweighted()

This method selects an atom from the currently active material, based only on the stoichiometry of the material. Weighting the selection by the scattering cross section would result in double-counting the weight, so it is not done.

Class ScreenedNuclearRecoil

The methods documented below are the public methods of the class which are directly useful to the end user for setting physics parameters. The main PostStep-DoIt() method implements the algorithm described in the rest of the paper, and is only used by GEANT4 internals.

*Method: ScreenedNuclearRecoil(const G4String& processName = "ScreenedElastic", const G4String &ScreeningKey = "zbl", G4bool GenerateRecoils = 1, G4double RecoilCutoff = 100.0*eV, G4double PhysicsCutoff = 10.0*eV)*

The constructor for this process allows the user to set a number of important physics parameters.

ScreeningKey selects which screening function will be requested from the external PYTHON module which generates screening tables and cross sections

GenerateRecoils controls whether recoil particles are generated and tracked, or whether a local energy deposition is made with the energy that would otherwise have been transferred to a recoil particle.

RecoilCutoff sets the energy below which a recoil will not be generated, and below which an incoming particle will be stopped with no further interaction. The stopped particles deposit energy (if permitted), and are allowed to decay if appropriate (“stop-but-alive” if any atRest processes exist, otherwise “stop-and-kill”).

PhysicsCutoff sets the energy cutoff used in the calculation of the total scattering cross-section, as described above. Its value is typically set to between 1 eV and 10 eV for problems in which forward multiple scattering is important. For problems involving backscattering, it can be raised to 100 eV or beyond to improve efficiency. Changing this parameter changes the mean-free-path and should not have a strong effect, unless the mean-free-path is approaching the length scale of the material in which the particle is traveling.

Method: AllowEnergyDeposition(G4bool flag)

If this is called with a flag of zero or false, all calls to deposit local energy are suppressed, but all processes proceed normally otherwise. This is useful for measuring how much energy is deposited as a result of nuclear collisions. Note that this leaves

the rest of the physics and random number consumption strictly alone, so that by resetting the random number generation, one can run exactly the same events with this on and off, and subtract the results to see how much energy was deposited in final stopping of particles when they reach the RECOILCUTOFF energy described above.

Method: EnableRecoils(G4bool flag)

This dynamically controls the same variable set by GENERATERECOILS in the constructor. The value can be changed at any time.

Method: SetMFPScaling(G4double scale)

This allows the mean-free-path computed from $l_\mu = 1/N\sigma_0$ to be scaled by an arbitrary amount, in a consistent way so that the underlying physics isn't changed. It is intended to improve tracking of particles in thin foils, where the thickness of the foil is less than a few times the mean-free-path. It can be changed at any time (e.g. one could add to a stepping action code to change it in a thin foil, and then reset it for better efficiency in regions with longer scale lengths).

Method: SetRecoilCutoff(G4double energy)

This dynamically controls the same variable set by RECOILCUTOFF in the constructor, and can be changed at any time.

Method: SetPhysicsCutoff(G4double energy)

This dynamically controls the same variable set by PHYSICSCUTOFF in the constructor. Although it can be changed at any time, there is a relatively high cost associated with doing so, since the physics tables for this process must then be reloaded. It is intended to allow the user to change it between runs, without restarting the GEANT4 kernel.

Method: SetCrossSectionHardening(G4double fraction, G4double HardeningFactor)

This enables the cross-section enhancement algorithm described above. A subset of the interactions, with probability FRACTION, has its cross-section increased by a scale of HARDENINGFACTOR by reducing the impact parameter appropriately. It can be changed at any time.

Method: G4double GetNIEL()

This returns the total energy which has been deposited as local energy depositions by this process in the most recent step. It is reset at the start of each step, so it must be accessed in the UserSteppingAction or in a subclass which overrides PostStep-DoIt() if its value is of interest. It is assumed to represent the Non-Ionizing Energy Loss (NIEL) if the RECOILCUTOFF is set low enough that essentially all of the remaining energy in a particle will be deposited collisionally. This value is valid whether ALLOWENERGYDEPOSITION is true or false.

References

- [1] J. P. Biersack, L. G. Haggmark, A Monte Carlo computer program for the transport of energetic ions in amorphous targets, Nucl. Instr. and Meth. in Physics Res. 174 (1980) 257–269.
- [2] J. F. Ziegler, J. M. Manoyan, The stopping of ions in compounds, Nucl. Instr. and Meth. in Physics Res. B35 (1988) 215–228.
- [3] SRIM reference website (2004).
URL <http://www.srim.org>
- [4] S. Agostinelli, et al., GEANT4—a simulation toolkit, Nucl. Instr. and Meth. in Physics Res. A506 (2003) 250–303.
- [5] GEANT4 reference website (2004).
URL <http://geant4.web.cern.ch/geant4/>
- [6] J. F. Ziegler, J. P. Biersack, U. Littmark, The Stopping and Range of Ions in Solids, Pergamon Press, New York, 1985, p. 56.
- [7] J. F. Ziegler, J. P. Biersack, U. Littmark, op. cit., 1985, p. 48.
- [8] M. H. Mendenhall, R. A. Weller, Algorithms for the rapid computation of classical cross sections for screened coulomb collisions, Nucl. Instr. and Meth. in Physics Res. B58 (1991) 11–17.
- [9] R. Franich, P. Johnston, I. Bubb, Efficient Monte Carlo simulation of heavy ion elastic recoil detection analysis spectra, Nucl. Instr. and Meth. in Physics Res. B219-220 (2004) 87–94.
- [10] P. Pusa, T. Ahlgren, E. Rauhala, Fast Monte Carlo simulation for elastic ion backscattering, Nucl. Instr. and Meth. in Physics Res. B219-220 (2004) 95–98.
- [11] T. S. Taylor, The range and ionization of the alpha particles in simple gases, Phil. Mag. 26 (1913) 402–410.
- [12] M. H. Mendenhall, R. A. Weller, An algorithm for ab initio computation of small-angle multiple scattering angular distributions, Nucl. Instr. and Meth. in Physics Res. B93 (1994) 5–10.

- [13] H. W. Lewis, Multiple scattering in an infinite medium, *Physical Review* 78 (5) (1950) 526–529.
- [14] M. Abramowitz, I. Stegun (Eds.), *Handbook of Mathematical Functions*, Dover, New York, 1965, pp. 888, 920.
- [15] PYTHON reference website (2004).
URL <http://www.python.org>