Description of the Medley Code:
Monte Carlo Simulation of the Medley Setup

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INTRODUCTION

Neutron-induced charged-particle production, i.e., reactions like (n,xp), (n,xd), (n,xt), (n,x3He) and (n,xα), yields a large and relatively poorly known contribution to the dose delivered in fast-neutron cancer therapy. At the The Svedberg Laboratory (TSL) in Uppsala, a project is underway to measure these cross sections with a precision required for clinical use.

For this purpose, an experimental facility, MEDLEY, is under commissioning. It consists of eight detector telescopes, each being a Si-Si-CsI detector combination. This general design has been selected because it provides reasonable performance over the very wide dynamic range required to detect particles ranging from 5 MeV α particles to 100 MeV protons. A general problem in this kind of experiments is to characterize the response of the detection system. The MEDLEY code has been developed for this purpose.

Experimental studies of these kinds of charged-particle reactions show specific features. Some of these need to be optimized by means of, for instance, computer codes, prior to the measurement if good data are to be achieved.

Basically, charged particles lose energy along their paths by interactions with the electrons of the material. Particles with low energy or with high specific energy loss are easily absorbed. Systems, which use thick charged-particle production targets to gain desirable count rate, can then detect only charged particles with enough energy to escape the target. Thus, using a thick target results in a degraded energy resolution, and particle losses. Thin targets are required to provide better resolution, but at the cost of low count rates.

Registration of the entire energy of the particles reaching the detection system is also an ultimate goal. However, charged particles can interact with detection materials via nuclear reactions, which could result in other species of particles. From the detection point of view, the primary particles are lost and replaced by new types of particles, which may behave differently from their predecessors.

It is well known that charged particles traveling in a medium are deflected by many small-angle scatterings. This so-called multiple scattering can be described with a statistical distribution. The fluctuations in energy loss per step, called energy-loss straggling, are modeled in the same way, i.e., assuming a statistical behavior.

To get an acceptable neutron beam intensity, a rather thick neutron production target (2-8 mm) is required. This causes an energy spread of the incident neutron beam. In our case, the spread after a 4 mm thick 7Li target for neutron production is of the order of about 2 MeV.
To analyze the data and determine the true double-differential cross sections, the above mentioned effects have to be taken into consideration. We have therefore developed a Monte Carlo code, MEDLEY, in FORTRAN language, to simulate the experimental setup taking all relevant physical characteristics into account. In the MEDLEY code, particles, chosen from a given distribution, are followed through the detection system. The particle distribution is obtained by applying a stripping method to the measured spectrum supplied by a user. When the result from the MEDLEY code is in good agreement with the experimental data, the true double-differential cross sections is obtained. If needed, the correction procedure can be iterated. This iteration is performed until the above condition is satisfied.

This report presents the features included in the code, and some results. We compare our results with those from others where available.

EXPERIMENTAL SETUP
The neutron beam is produced by the $^7\text{Li}(p,n)^7\text{Be}$ reaction at $0^\circ$. It is defined by a collimating system of more than 4 m of iron and concrete. The beam at the target position is about 7 cm in diameter. A detailed description of the facility can be found in [1].

The charged-particle production targets are kept small so that to obtain not too large angular spread. The target thickness is in the order of a few hundreds of microns.

The experimental setup [2] consists of a 90 cm diameter vacuum chamber with eight $\Delta E-\Delta E-E$ telescopes, placed at different angles, four in the forward hemisphere and four in the backward. Figure 1 shows the chamber with the eight telescopes. In each telescope, the two $\Delta E$ detectors are totally depleted surface barrier silicon detectors and the $E$ detector is a CsI(Tl) crystal. The first silicon detector is either 50 or 60 $\mu$m thick. The second one is 400 or 500 $\mu$m thick. All silicon detectors have an active area of 450 mm$^2$. The CsI(Tl) detector is a 30 mm long cylinder with a diameter of 40 mm. The crystals are tapered to 18 mm diameter to match a Hamamatsu S3204-03 photodiode. This conical cylinder is 20 mm long. Figure 2 shows the arrangement of the detectors in the telescope.

Each set of detectors is put inside an aluminium housing with an opening area slightly larger than the active area of the silicon detectors. The housings are then mounted on rails. The target-to-detector distance can be varied from 15 to 25 centimeters. The symmetry line of the telescope is aligned to point at the centre of the target.
**Figure 1:** The scattering chamber and the arrangement of the telescopes.

![Diagram of scattering chamber and telescopes](image)

**Figure 2:** The arrangement of the measurement simulated in the code.

![Diagram simulating measurement](image)
CODE STRUCTURE
The MEDLEY code, written in FORTRAN, is composed of two major parts. The first part is used to construct the true double differential cross section (DDX) data from which the particles will be sampled. This true DDX spectrum is obtained by using a stripping method to the user-supplied measured spectrum. A particle is then followed in the system until its history ends. After the particle track has been terminated, information registered in the detecting material is recorded. This procedure resembles what actually happens during the experiment. The information obtained in this way is then compared with the measured spectrum. If the result from the code does not agree with the experimental data, an adjustment to the true DDX spectra is conducted. The code repeats the calculation again and continues the iteration procedure until a reasonable agreement is reached. With a moderate development, the code can achieve such a level within a few iterations. This part is not using the Monte Carlo technique, but is implemented to help the user getting the true DDX without bothering about a complicated matrix technique.

Once the particle is picked up from the given distribution, it will be transported through all materials of the detection system. So, in the second part of the code, the corrections mentioned earlier, such as energy loss in the material, losses due to nuclear reactions, multiple scattering, angle straggling, and energy loss straggling, are taken into account, using a Monte Carlo technique.

The code follows one particle type per run and only one angle per run. The user can get the full description of the measurement by adding information from several runs.

The code works in several steps:
1) Read input information such as stopping-power values, geometrical parameters and measured spectrum.
2) Construct a trial true DDX spectrum from the user-given measured data.
3) Perform the Monte Carlo simulation for the given number of particles.
4) Compare the result with the given experimental data. Adjust the DDX spectrum if necessary, and run another iteration.
5) Print the calculated data. The code stores energy deposited in all geometrical bodies implemented in the code, e.g., the target, the two Si detectors, and the CsI.

The general and detailed flowcharts of the code are shown in figures 3 and 4, respectively.
1. Input

Necessary code inputs are stopping power values and charged-particle reaction cross sections for the materials that are used in the experimental setup [2]: C, Si, Al, CsI, CH₂, SiO₂, Si₃N₄. Since the code handles protons, deuterons, tritons, ³He and ⁴He ions, data for all particle types are read in at the start of each run. In addition, the energy spectrum of the charged particles measured in the neutron reactions is read into the program together with parameters of the geometrical setup.

2. Construction of the true DDX

Using a stripping procedure on the measured spectrum, a trial true spectrum is constructed. A beam of mono-energetic particles looses energy in the target. Therefore, the counts in the highest energy bin are too low due to the spread of particles down to lower energy bins. The counts in the highest bin have therefore to be increased according to

$$C_{new} = C_{old} \times \frac{Energy loss}{Binwidth}$$

Accordingly, the counts, which are added up to that bin, are taken away from the corresponding bin below. Then the procedure continues with the next bins covered by the loss.
3. Monte Carlo simulation
The reaction depth in the target is sampled using a rectangular distribution, i.e., all points in the target are equally probable, thus assuming that the incident neutron beam is not attenuated. With the actual target thicknesses, this is a very good approximation. From the reaction point, a direction towards the telescope is selected using the differential cross section data. If the sampled direction points to the detector surface, the particle direction is accepted and the energy of the charged particle is sampled, again using the double differential cross section data.

The charged-particle energy loss while passing through the target is calculated. Energy-loss straggling and nuclear reaction probabilities are considered. The models used to simulate multiple scattering, energy-loss straggling, and nuclear reaction probabilities are explained below. From the target to the first Si-detector, the particle does not lose any energy since there is vacuum.

In the silicon detectors, the energy loss, energy-loss straggling and nuclear reaction probabilities are considered but the angular straggling is neglected. A motivation for not including multiple scattering in the ΔE-detectors is that it will not affect the path length, and therefore the deposited energy in the ΔE-detector, enough to be considered.

In the CsI detector, the transport is carried out by moving the particle stepwise. The step length corresponds to some predefined fractional energy loss, typically 8.3 % per step. (The reason for this choice is described below). The energy loss for each step is corrected for energy-loss straggling and nuclear reactions. If a nuclear reaction occurs, the particle energy is deposited at the point of interaction, the particle is lost and a new particle is sampled in the target. For each step, the angular deflection caused by multiple scattering is sampled from a Gaussian distribution. The cutoff energy for particle transport is set to 5 MeV and if the particle energy is below 5 MeV, the particle is considered absorbed at that point.

4. Comparison and correction
The output spectrum from the code is compared with the measured spectrum. A least-square fit is applied to check whether the calculated result is in good agreement with the experimental one. If the difference is larger than acceptable, the first DDX data is adjusted. The adjustment is done by calculating the ratio between the calculated (output from the code) and the measured spectrum bin by bin. This ratio is correspondingly applied to the DDX data. This newly adjusted DDX data is then fed as a new input DDX data to the code.

5. Output from the code
The output from the code is stored on an event-by-event basis, as is the data from the experiment. The parameters stored are the energy at the creation point, and the energies deposited in the target, the first and second ΔE-detector, and the CsI detector, respectively. From this information, the input spectrum and the calculated spectrum is post-processed using external programs.
Figure 4: The flow structure of the Monte Carlo section in the code.

Physics
1. Multiple scattering
Heavy charged particles traversing a medium are deflected by many small-angle scatterings. The principal contributor to these deflections is Coulomb scattering from the screened nuclei. Since the angular deflections after each step is the net result of many, from each other independent, small deflections, the total deflection \( \theta \) can be considered Gaussian-shaped distributed and the multiple scattering angular distribution approximated using a Gaussian distribution [3, 4]. For large-angle deflections, the Gaussian shape cannot sufficiently well describe the angular deflection. However, there is only a small probability that the particle will
scatter into a large angle (1-2%) and escape the system due to this effect. Therefore, using a Gaussian distribution will not seriously affect the desired results.

In analogy with the stopping power, where the energy loss is proportional to the thickness of the traversed medium, the mean square scattering angle increases linearly with increasing thickness of the traversed medium. If we assume that the energy during the step is constant, the mean square scattering angle per unit length of traversal is constant, and the root-mean-square scattering angle per step can be considered proportional to the step length. The step length \( dl \) is, in a homogenous medium, directly proportional to the number of targets, i.e., number of collisions.

Thus,
\[
\frac{d\theta^2}{dl} = Tdl
\]
\[
\frac{T}{\rho} = \frac{1}{\rho} \frac{d\theta^2}{dl}
\]

where \( T/\rho \) is called the mass scattering power (\( \rho \) is the density of the medium) and \( \overline{\theta}^2 \) is the mean square scattering angle.

The mean square scattering angle of the Gaussian distribution is calculated using [3,4]:
\[
T = \left( \frac{4\pi}{\alpha} \frac{m_c}{\beta \rho} \right)^2 \frac{1}{X_o} = \left( \frac{21.2 \text{MeV}}{E_i} \right)^2 \frac{1}{X_o} = \left( \frac{10.6 \text{MeV}}{E_i} \right)^2 \frac{1}{X_o} \Rightarrow
\]
\[
\overline{\theta}^2 = \left( \frac{10.6 \text{MeV}}{E_i} \right)^2 \frac{x}{X_o}
\]

where \( E_i \) is the particle kinetic energy, \( X_o \) is the radiation length and \( x \) is the step length [4].

\( X_o \) is calculated using:
\[
\frac{1}{X_o} = \frac{4\alpha}{A} \sum \frac{w_j}{X_j} \ln(183Z^{1/3})
\]
\[
\frac{1}{X_o} = \sum \frac{w_j}{X_j}
\]

where \( w_j \) is the weight percent of a material when calculating \( X_o \) for a certain composition. The calculated values of \( X_o \) for the materials of interest are presented in table 1.
Table 1: The radiation length $X_0$ for some materials.

<table>
<thead>
<tr>
<th>Material</th>
<th>$X_0$ [g/cm$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CsI</td>
<td>8.11</td>
</tr>
<tr>
<td>C</td>
<td>44.6</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>47.1</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>27.7</td>
</tr>
<tr>
<td>Si$_3$N$_4$</td>
<td>26.9</td>
</tr>
</tbody>
</table>

Having the information regarding the width of the distribution, the scattering angle is sampled using a (non-normalized) Gaussian distribution:

$$P(\theta)d\theta = 2\frac{\theta}{\theta^2}e^{-\frac{\theta^2}{2\sigma^2}}d\theta = 2\frac{\theta}{\theta^2}e^{-\frac{\theta^2}{2\sigma^2}}d\theta.$$  

This is true since $\bar{\theta} = 0$, i.e., there are as many scatterings into $+d\theta$ as into $-d\theta$ with the net result zero.

2. Energy loss

The step length is calculated using fractional energy losses:

$$E_{n+1} = E_n \times 2^{-k}.$$  

$$\text{Step length} = \frac{E_{n+1} - E_n}{\frac{dE}{dx}}.$$  

$E_n$ is the energy at the beginning of step $n$ and $E_{n+1}$ is the energy after the step; $k$ is set to 8 leading to a fractional energy loss corresponding to about 8.3% per step. The step length is then just the energy loss divided by the stopping power at the mean energy during the step.

3. Energy loss straggling

The result from energy loss calculations using stopping power does only yield the average behaviour of the particles. In practice, there is a fluctuation in energy losses, given by [3],

$$\sigma^2 = \langle (E - \langle E \rangle)^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2,$$

where $\langle E \rangle$ is the mean energy loss calculated using stopping power. Now, during each step, $n$ number of collisions will occur and at each collision the energy $E_r$, which is very small, will be lost. The number of collisions is distributed as

$$\langle n - \langle n \rangle \rangle = \langle n \rangle,$$

where $\langle n \rangle = N \int \sigma_{ij} \, dx$. We thus get

$$\langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{P} \sum_{i=1}^{P} \langle n^i \rangle E_r - \langle n \rangle E_r \rangle^2 = \ldots = N \sum \int \sigma_{ij} E_r^2 \, dx.$$
By using a somewhat simplified model for the stopping power, we have

\[- \frac{dE}{dx} = N \sum \sigma(E) E = \frac{4\pi z^2 e^4}{mv^2} \int \frac{db}{b} \cdot \]

\(E\), and the impact parameter, \(b\), are related by

\[E_r = \frac{2\pi z^2 e^4}{mv^2 b^2} \frac{dE}{E} = -\frac{2db}{b} \cdot \]

Now if we set \(E_{\text{max}} = \frac{mv^2}{2}\) and \(E_{\text{min}} = 0\), we get

\[\int dE \left( E^2 - \left( \frac{E_{\text{max}}}{E_{\text{min}}} \right)^2 \right) = N \sum \sigma E_r^2 = \frac{2\pi z^2 e^4 NZ E_{\text{max}}}{mv^2} dE = 4\pi z^2 e^4 NZ \Rightarrow \]

\[\sigma_x = 2\pi z^4 \sqrt{NZ \Delta x} \cdot \]

All calculations of energy loss include corrections for energy loss straggling. The Gaussian distribution used is valid for all particles considered, e.g., p, d, t, ^3He and ^4He up to about 20 MeV [6]. Above 20 MeV, the Gaussian distribution underestimates large energy losses but the effect of this simplification is not considered to be decisive. At high energies, the particles are more likely to pass through the \(\Delta E\)-detectors and thus deposit their remaining energy in the CsI. Therefore, the underestimation of large energy losses can only prolong the range of the particle in the CsI. It is very unlikely that this should cause any differences in the total absorbed energy in the CsI since the range of the particles is less than the size of the detector. The width of the Gaussian is calculated using the equation above, which in another form, \(\text{FWHM}=2.35 \sigma_x\), is also given by in ref. [6], in case of silicon:

\[\text{FWHM} = 10.1 z \sqrt{\Delta x} \cdot \]

This gives the FWHM in keV, \(z\) is the atomic number of the particle and \(\Delta x\) is the step length in \(\mu m\).

4. Nuclear reactions

When heavy charged particles pass through matter they do not only lose energy through Coulomb scattering with electrons or deviate from the straight line via multiple scattering with the screened nucleus. A more dramatic possibility is that the particle strikes a nucleus and a nuclear reaction occurs. Some possible reactions are elastic scattering, inelastic scattering and capture reactions. In the code, the total reaction cross section is considered and if a nuclear reaction occurs the particle is assumed to be lost and all its energy, not including energy released during the reaction, is deposited at the interaction point. The total reaction cross section can be expressed in a simple way using geometrical arguments [7]:

\[\sigma_x = \pi \left( R_p^2 + \frac{r_0 A^{1/3}}{2} \right)^2 \cdot \]

where \(R_p\) represents the proton projectile radius and the term \(r_0 A^{1/3}\) refers to the target nucleus radius. Now \(R_p\) and \(r_0\) are used as phenomenological fitting parameters to the cross
section data, where $R_p$ is allowed to be energy-dependent. These data are taken from [7] and are used to calculate the probability for a reaction to take place during the step. If a reaction occur, then the actual reaction point is taken to be $\rho \times$ step-length from the last step-point, where $\rho$ is a random number $[0,1)$.

RESULTS AND COMPARISONS
We have simulated the response function of the telescope to alpha particles. The telescope consists of a 50 $\mu$m, a 500 $\mu$m silicon detectors and a 3 cm CsI(Tl) detector. The telescope, placed at 20° scattering angle, detects alpha particles emitting from a 4.1 mg/cm$^2$ carbon target tilted 20 degrees with respect to the beam. For this demonstration, we have produced pseudo-data, a flat energy distribution of alpha particles extending from 0 up to a maximum energy of 80 MeV. The result is shown in figure 5. The energy resolution of the system at 50 MeV is about 1 MeV and about 3 MeV at 8 MeV. The main contribution to the resolution is from the energy loss of alphas in the target.
Figure 5: A response function of a telescope to alpha particles with the flat distribution from 0 up to 80 MeV. The telescope consists of a 50 µm and a 500 µm silicon detector, and a 3 cm CsI(Tl) detector.

Next test was provided by an analysis of real data. For this, we have used the $^{12}$C(n,xα) reaction at 39.7 MeV beam energy at an angle of 20°, measured by Johnson et al. [8]. As a first test, we have studied the effect of the stripping method alone. The input DDX spectrum of the code is constructed by using the stripping method. Counts from lower energy bins, covered by the energy loss, are stripped and added back to the original bin. Figure 6 illustrates the result obtained using this method. We have used the measured data as our user-supplied spectrum and their corrected spectrum to compare with our results. The stripping method works very well at the high-energy end of the spectrum, but is not in a very good agreement at the low-energy end. A smoothing function needs to be applied to the low-energy end of our corrected spectrum.
Figure 6: An at-reaction-point (corrected) and an after-target (uncorrected) double differential cross section of the $^{12}$C(n,x$\alpha$) reaction for 39.7 MeV neutrons at angle of 20°. The target thickness is 4.1 mg/cm$^2$.

As a second step, we have tested our full particle transport. Since our procedure is in a reverse direction to their strategy, we have, therefore, used their corrected data as an input spectrum to our program and compared our result with their uncorrected data. The result is satisfactory and is shown in figure 7.
\[ C(n, x_\alpha), \ E_n = 39.7 \text{ MeV at 20 degrees} \]

Figure 7: An at-reaction-point (corrected) and an after-target (uncorrected) double differential cross section of the \(^{12}\text{C}(n,x_\alpha)\) reaction for 39.7 MeV neutron at angle of 20°. The target thickness is 4.1 mg/cm\(^2\).

CONCLUSION AND FUTURE WORK

We have developed a code, MEDLEY, partly using a Monte Carlo technique, to correct for distortions of the initial energy spectrum due to energy loss in the target, multiple scattering, energy loss straggling and losses due to nuclear reactions during the course from the production to the measured point. The code generates the true double differential cross section spectrum for the given experimental spectrum and the detection configuration.

The other procedure in use in the program is the extraction of the true double differential cross section data by applying the correction method to the measured data and, if necessary, an iteration mechanism without involving complex methods.

We have simulated the response function of our telescope to alpha particles. The response function is well understood. The predicted energy resolution of the telescope of a 50 µm, a 500 µm silicon detector and a 3 cm Cd(Tl) detector is about 3 and 8 MeV at 1 and 50 MeV alpha, respectively. We have found that the major source of the energy spread in the telescope is from the energy loss in the target.
Also, we have tested our stripping method to construct the double-differential cross section data using the measured spectrum from the user as a starting point. The method works very well at the high-energy end of the spectrum but is overestimating the data at the low-energy end. A smoothing function should be applied to the low-energy end. This task remains to be done.

For the comparison, we have used the data presented by Johnson et al. [8]. The code has reproduced the results well.

The user, in the end, will be able to “switch on” each effect individually. The consequence from each source can be clearly followed one by one. The user can then minimize sources of distortion afterwards. The use of the code in this way will be an important help in optimizing experiments of this kind.

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