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Title: DETERMINISTIC PROTON TRANSPORT SOLVING A ONE DIMENSIONAL FOKKER-PLANCK EQUATION

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Deterministic Proton Transport Solving a One Dimensional Fokker-Planck Equation

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Abstract:

The transport of protons through matter is characterized by many interactions which cause small deflections and slight energy losses. The few which are catastrophic or cause large angle scatterings can be viewed as extinction for many applications. The transport of protons at this level of approximation can be described by a Fokker-Planck equation. This equation is solved using a deterministic multigroup differencing scheme with a highly resolved set of discrete ordinates centered around the beam direction which is adequate to properly account for deflections and energy losses due to multiple Coulomb scattering. Comparisons with LAHET for a large variety of problems ranging from 800 MeV protons on a copper step wedge to 10 GeV protons on a sandwich of material are presented. The good agreement with the MonteCarlo code shows that the solution method is robust and useful for approximate solutions of selected proton transport problems.

1.0 Introduction:

The basic purpose of this paper is to present an evaluation of the possible use of an advanced discrete ordinates code in the calculation of the attenuation, emergent average energy, angular spreading and energy spreading of broad proton beams which have passed through a given amount of material. It is shown that the discrete ordinates method used in the one dimensional ONEBFP charged particle transport code can accurately calculate the attenuation, emergent average energy, and angular spreading for plane wave proton beams in a minimum amount of computation time. A similar conclusion for the calculation of energy spreading of the beam could not be reached within the time scale of this study.

Another critical element of this paper has been the identification of the sensitivity of the results to changes in cross sections. Our literature search showed that there was a wide variation in the cross section data used with different transport codes were found. Initial comparisons with LAHET, a monte carlo code commonly used for purposes such as this application, showed about the same beam attenuation, but showed significant disagreement in the angular dispersion of the beam as well as minor differences in other quantities. The dispersion disagreement was tracked to differing scattering models used in the two codes. Differences in the other quantities were traced to noticeable differences in appropriate cross sections. A single comparison to another monte carlo code named TRIM also indicated differences in the small angle scattering model. Its results agreed with neither ONEBFP nor the LAHET models.

ONEBFP used values from a published compilation of calculated cross section data by J. Janni (ref. 4). LAHET calculates cross sections on the fly from built-in cross section models. However, when both codes were manually given the same cross section data, they produced the same results.

This study indicates the need for integral experimental or other validation of the cross section data to be used for the proton radiography application.

2.0 ONEBFP Code Methods:

The ONEBFP[1] code originated with the work of Walters on the linear nodal method[2]. He outlined a method that solved the Boltzmann equation shown below for two space dimensions.

$$\mu\frac{\partial}{\partial x}\Psi(x, y, E, \Omega) + \eta\frac{\partial}{\partial y}\Psi(x, y, E, \Omega) + \sigma_{total}\ \Psi(x, y, E, \Omega)$$
$$= Q(x, y, E \leftarrow E', Q \leftarrow Q') + Q_{ex}(x, y, E, \Omega)$$

where $\Psi(x,y,E,\Omega)$ is the angular flux at energy E at location (x,y) in direction Ω. The direction cosines for that direction relative to the x and y axes are, respectively, μ and η.

σ_{total} is the total cross section for all reactions that remove particles from the differential element at (x,y,E,Ω). It includes absorptions and scatters to other energies and angles.

And, finally, $Q(x,y,E\leftarrow E',\Omega\leftarrow\Omega')$ is the source of particles arriving at energy E in the direction Ω by scatters from angle Ω' and energy E'. $Q_{ex}(x,y,E,\Omega)$ is the contribution from any external fixed source.

One obtains the Fokker Planck equation by assuming that the scattering of charged particles is highly forwardly peaked and performing an associated asymptotic expansion. To lowest order, this expansion produces the following transport equation in 1-d slab geometry. For convenience, we drop the notation (x,y,E,Ω) with the understanding that the dependencies are still there.

$$\mu\frac{\partial\Psi}{\partial x} - S\frac{\partial\Psi}{\partial E} + \sigma_{rem}\Psi = Q_{ex} + \frac{K}{2}\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial\Psi}{\partial\mu}$$

where S is the stopping power of the medium and is a function of the inelastic cross section. K is the transverse momentum transfer and is a function of the elastic cross section. σ_{rem} is σ_{total} minus the scattering losses. The term involving S on the left side of the equation accounts for changes in energy and the term involving K on the right side accounts for changes in direction.

Note that equation (2) is of the form of the two space dimension Boltzmann equation shown in equation (1), with y replaced with E and η replaced with -S. We should thus be able to solve the Fokker Planck equation in one space dimension and the energy dimension using the two dimensional spatial discretization of Walters.

When we discretize (mesh) the angular variable in the transport equation using the method of Morel[3], we obtain the following form for the equation that ONEBFP solves.

$$\mu_m \frac{\partial \psi_m}{\partial x} - S\frac{\partial \psi_m}{\partial E} + \left[\sigma_{rem} + \frac{K}{2w_m}\left(\frac{\alpha_{m+1/2}}{\mu_{m+1}-\mu_m} + \frac{\alpha_{m-1/2}}{\mu_m - \mu_{m-1}}\right)\right]\psi_m =$$

$$Q_m + \frac{K}{2w_m}\left(\frac{\alpha_{m+1/2}}{\mu_{m+1}-\mu_m}\psi_{m+1} + \frac{\alpha_{m-1/2}}{\mu_m - \mu_{m-1}}\psi_{m-1}\right)$$

where

$$\alpha_{m+1/2} + \alpha_{m-1/2} = -w_m\mu_m \;; \qquad \alpha_{1/2} = 0$$

and μ_m is the direction cosine of the discrete direction m, ψ_m is the angular flux in that direction, w_m is the quadrature weight associated with the direction, Q_m is the component of Q_{ex} in the direction m, and the alpha terms are functions solely of the angular mesh structure at, respectively, the left and right edges of the angular interval m.

Note that this equation is still in the form of the original Boltzmann equation but that there is an effective total cross section given by the term in square brackets. It is composed of σ_{rem} and a term representing the scattering from direction m to other directions. There is also an effective source given by the terms on the right side of the equal sign. The second of these terms represents the scattering into direction m from other directions. ONEBFP explicitly forms these effective terms internally. They are not included in the cross section data, per se, as in some other codes.

The discretization of the space and energy variables follows that described by Walters[2]. There is a second order term ignored in the foregoing description that we shall now address. In deriving equation (2), there was a Taylor's series expansion used and only the first term of the expansion was used. One really needs to include the second order term in order to accurately calculate the energy loss straggling. We approximate that energy diffusion term by appending an additional term to the source which shows up in the fully discretized equation as a transfer from the angular flux in direction m in any energy group to the same direction in the next lower energy group. This term is included in the ONEBFP code but was not used in this study.

It should be noted that ONEBFP obtains its cross sections from an external file and does not generate them from internal models. The user supplies the quantities S, K, σ_{rem}, and the second order scattering cross section in that database.

3.0 Code Description:

The ONEBFP user must establish a mesh structure in space, angle, and energy for the calculation. A special feature in the code is to specify a logarithmic varying mesh in angle. This mesh is constructed to give fine resolution in the angles in the neighborhood of the beam direction with a gradually coarser mesh in the directions away from the beam. The energy mesh is designed to represent the energy variation in the cross sections as well as to capture the beam spreading in enrgy as it is trasported through the medium. The spatial mesh is the least sensitive parameter as long as the mesh spacing is in the neighborhood of one mean free path or smaller. As indicated below, our parametric studies demonstrate that when reasonably sized meshes are chosen for each of the variables, the calculations made in this application are accurate.

These meshes lead to running times in the few seconds to minutes range on an IBM RISC6000 model 590 workstation.

On an academic note, ONEBFP can generate individual negative fluxes in off peak (in energy) areas when the beam is almost monoenergetic. This is most likely due to the energy differencing scheme used in the ONEBFP code. This is a problem commonly seen when there are steep gradients in the calculated particle density. The problem disappears when source energy distributions representative of proposed designs are used as there are then not such steep gradients in energy.

In addition to the comparisons to other transport codes, we calculated the results for five benchmark calculations, three of which represent experiments or proposed experiments for which experimental results are not yet available. These results are found in Appendix E.

4.0 Evaluation of Code Capability:

Parametric studies to determine adequate meshing were performed for a wide variety of problems. We focussed on the calculation of:

1. The attenuation of the beam current.

2. The average energy of the exit beam.

3. The angular distribution of the exit beam.

4. The energy spread, or spectrum, of the exit beam.

The ONEBFP user must establish a mesh structure in space, angle, and energy for the calculation. The mesh must be fine enough in each of these variables to resolve the structure in the flux solution. The adequacy of the mesh structure is determined by refining it until no significant differences in results are found. A series of runs were performed to validate the adequacy of the mesh structure(s) used in this study. Sixty angles arranged in the logarithmic pattern gave good angular resolution. A hundred spatial meshes gave good results for 100 grams per square centimeter of copper for both 10 GeV and 800 MeV protons. Even coarser spatial meshes are adequate in order to get only the angular distribution correctly. The angular distribution is also relatively insensitive to the energy mesh used.

In order to approximate a monodirectional beam source, we input source only in the most normally incident angular bin in the ONEBFP run. This is a good approximation as this angular bin is only 1.2 milliradians in width for the 60 angle set used in most of the calculations, whereas the exit beam is many milliradians in width. The source intensity within the bin is constant in angle. There is a unit input current for all the calculations.

The energy spectrum is sensitive to the number of energy groups used. An energy structure which resolves the incoming source spectrum is adequate for calculating the outgoing spectrum as might be expected, since in passing through the material, the beam has been spread in energy. In actual practice, the 10 GeV source is fairly broad, typically in the tens of MeV, so energy mesh intervals on the order of five MeV prove adequate. In the cases where we tried to model a monoenergetic source, we used an energy mesh with one MeV wide groups.

As ONEBFP is a one dimensional code (in space), we are limited to calculations for a source incident upon the surface of a slab of material. This slab can be thought of as a thickness of material with infinite lateral extent with no variation in the lateral direction. The incident source may have an angular distribution, that is, a variation with respect to the angle from the normal to the surface of the slab.

ONEBFP requires four key cross sections. They are the removal, the transverse momentum transfer, the stopping power, and a second order group downscattering term that largely dictates the energy loss straggling. We used Janni's nonelastic nuclear cross section for the removal, thus modeling these interactions as simply causing removal from the beam. It also means we do not generate or track any secondary particles from this reaction, but rather are concentrating on calculating the beam attenuation. The transverse momentum transfer cross section characterizes the small angle scattering. For it, we used Janni's relativistic Born value of the screened Rutherford scattering. Possible other small angle scattering, such as strong force scattering from the nucleus, should also be included in the transverse momentum transfer, but were ignored for this study because it was thought omission would cause a negligible effect. Janni gives the stopping power explicitly, so no modeling was needed there.

5.0 Results

Several problems were calculated with the ONEBFP code using the cross section data of Janni, and compared to LAHET or TRIM calculations. Each will be described below.

For all problems, the energy spectrum of the incident beam with a gaussian distribution of the form, $S(E) \sim \exp(-(E/a)^2)$, where E is the energy difference from the mean beam energy and a the width. For the 10 GeV sources, we used a value of 25 MeV for the parameter a in the expression. For the 800 MeV sources, we used a value of a that gives a full width at half maximum of 2 MeV.

For all comparisons it should be noted that the Monte Carlo codes, LAHET and TRIM, each initially using their own respective cross section models. Error bars are not shown for either LAHET or TRIM. For LAHET, the error is small and would not show graphically. In all the LAHET calculations, the Gaussian multiple scattering treatment was included as well as range straggling.

Figures 1 and 2 show comparisons of the ONEBFP and LAHET[8] calculations of the exit angular and energy distributions for 10 GeV protons normally incident on a slab copper 100 g per sq. cm thick (11.2 cm). ONEBFP used a linear interpolation of the Janni cross section data and LAHET used its internal cross section modeling. The exit total currents are about the same for both calculations. However, the ONEBFP calculations show considerably more angular dispersion than the LAHET results. The discrepancy in the angular distribution is explained by the methods that the codes account for the deflections due to small angle multiple scattering. In ONEBFP, that effect is dictated by the "transverse momentum transfer" cross section, which is taken from Janni's compilation for the relativistic screened Rutherford scattering. In LAHET, there are two components, the screened Rutherford scattering which uses a Gaussian multiple scattering treatment and single event elastic scattering from the nucleus. Both components are calculated from internal models. The single event elastic scattering is itself composed of two parts, the strong force scattering and the nuclear coulomb scattering.

We first concentrate on comparing the screened Rutherford scattering. We do that by turning off all the nuclear interactions in the LAHET calculation, thus getting rid of the single event elastic scattering from the nucleus, but also eliminating any attenuation of the beam. A comparison with a ONEBFP calculation, with its removal cross section set to zero to suppress the attenuation also, is shown in figure 3. Notice that there is still strong disagreement and since we have localized to the screened Rutherford scattering, we suspect differences in the data representing this reaction. Indeed, when a rough approximation of the Janni model for this reaction was built into the LAHET code, it produced fairly good agreement as shown in figure 4.

Most of the disagreement shown has now been explained by differences in the scattering models used in the cross section data. This is corroborated by arbitrarily adjusting the transverse momentum transfer cross section used by ONEBFP a small amount and achieving equally good agreement.

We now turn our attention to the average energy of the emergent beam. As you recall, it looked like LAHET showed a lower average energy than ONEBFP although it was a little hard to tell since ONEBFP exhibited the broad energy distribution derived from its broad source whereas LAHET used a monoenergetic source. The average exit energy is determined by the stopping power of the material through which the beam passes. We were

able to dump out the stopping power from the LAHET calculation and use it in the ONEBFP calculations. In order to more accurately show the position of the peak, we also arbitrarily narrowed the incident source in the ONEBFP calculation to 6 MeV. We also show ONEBFP results using Janni's value of the stopping power, this time using the narrow source. The results are shown in figure 5. There is approximate agreement on the location of the peak when both LAHET and ONEBFP use the same value of the stopping power.

A set of calculations using a source as nearly monoenergetic as possible in ONEBFP (all the source was put into one energy group of width one MeV at 10 GeV) and a monoenergetic source in LAHET were performed to assess the adequacy of the deterministic code to simulate energy loss of a beam. The two calculated exit spectra are shown in figure 6. The peaks do not align due to slight differences in stopping power. The exit beam has a narrower energy width in the ONEBFP calculation, indicating that all the energy straggling effects are not included. This is expected since ONEBFP omitted any energy loss straggling considerations. Also note that ONEBFP produces some non-physical, negative fluxes in the vicinity of the exit peak. This is thought to be due to the energy differencing scheme used in ONEBFP. That scheme is not guaranteed positive and when there are strong gradients of the solution in a problem, can generate negative fluxes. This effect arises in this comparison because of the attempt to handle a delta function in energy, that is, the monoenergetic source that was used in the LAHET calculations. When a sufficiently distributed source was used, no negative fluxes are generated. It should be noted that even when we get negative fluxes, there is particle balance, i.e. there are no particles lost due to this effect.

Finally, a lower proton beam energy was used to assess the feasibility of using this code for simulations of LANSCE experiments. The source was 800 MeV protons incident on the same 11.2 cm. thick slab of copper. Added to the comparison was another monte carlo code named TRIM which has a more single event scattering algorithm than ONEBFP or LAHET but may not be as extensively validated as LAHET at these energies. The attenuation was suppressed in the calculation. The exit angular and energy distributions are shown in figures 7 and 8. Note that the ONEBFP calculation used only 40 angles. At this energy, there is considerably more angular dispersion of the beam than at 10 GeV and a smaller number of angles is sufficient to resolve the angular distribution. TRIM calculates even less angular dispersion than LAHET. These differences are due to the small angle scattering models in the codes.

In the energy distribution shown in figure 8, note that the energy widths of the peak calculated by ONEBFP and TRIM are comparable, but the energy width calculated by LAHET is considerably narrower.

6.0 Conclusions:

The deterministic code, ONEBFP, has been shown to able to perform proton transport in one dimensional problems. The small angle multiple scattering is adequately calculated using the Fokker-Planck approximation of the transport equation with a logarithmic angular discretization. The spatial mesh need not be too fine for convergence of the calculation.

The angular dispersion is strongly impacted by the transverse momentum transfer, which shows the need for precise cross sections for a transport calculation. The emerging energy spectrum from slabs shows a numerical artifact of negative flux which may be ameliorated by a better energy differencing scheme. Finally, energy loss straggling has not been addressed in this paper, but should be available with an appropriate set of group to group transfer matrices.

7.0 References:

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4. J. F. Janni, "Proton Range-Energy Tables, 1keV - 10 GeV", Atomic Data and Nuclear Data Tables, 27, 2/3, (1982)

5. Richard E. Prael and Henry Lichtenstein, "User Guide to LCS: The LAHET Code System", LA-UR-89-3014, Los Alamos National Laboratory (September 1989).

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7. John Zumbro, Personal communication of typical beam energy width at 10 GeV

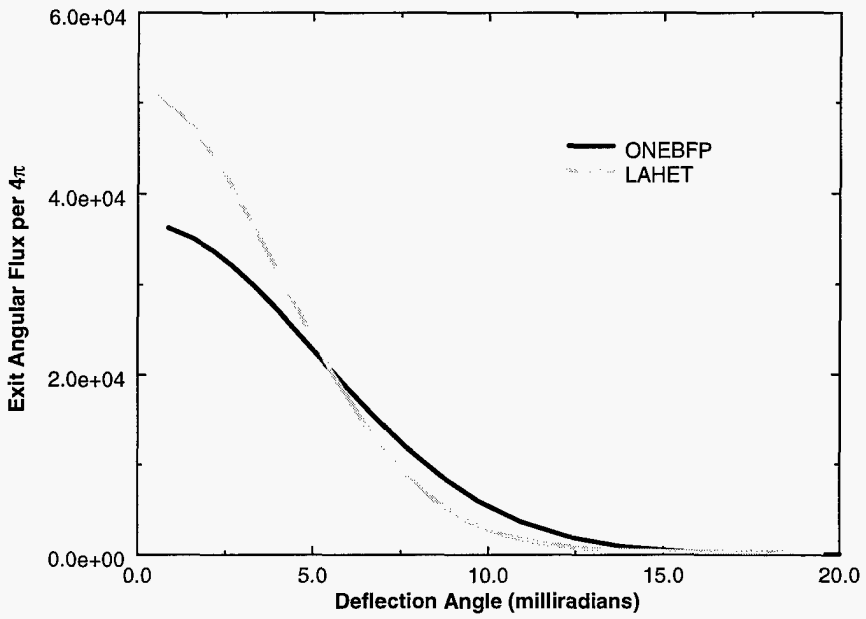

Figure 1: Comparison of ONEBFP and LAHET calculation of beam angular dispersion for 10 GeV protons normally incident on a 11.2 cm thick Copper slab. ONEBFP used 60 logarithmic spaced angular bins, 400 space zones, and 280 energy groups. LAHET is continuous.

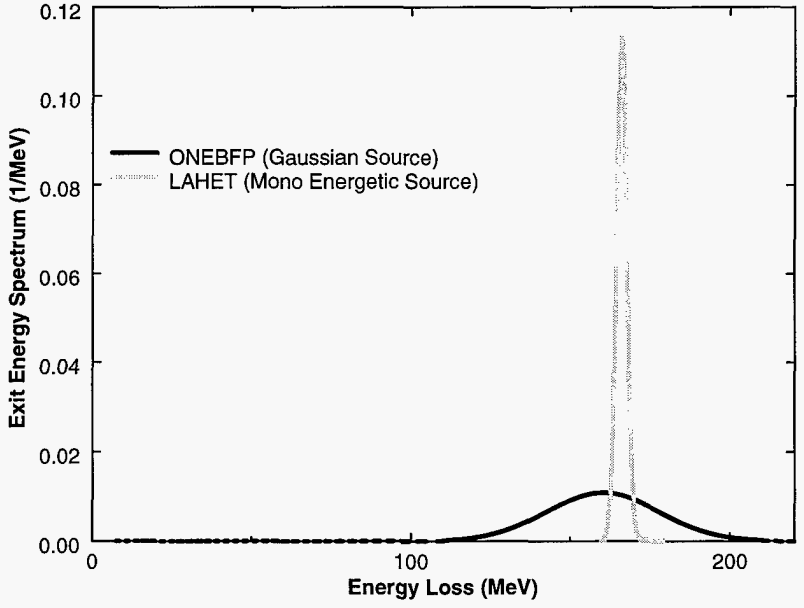

Figure 2: Comparison of ONEBFP and LAHET calculation of exit energy spectrum for protons normally incident on a 11.2 cm thick Copper slab. ONEBFP used a Gaussian energy source distribution 25 MeV wide cenetered on 10 GeV and LAHET had a monoenergetic source at 10 GeV.

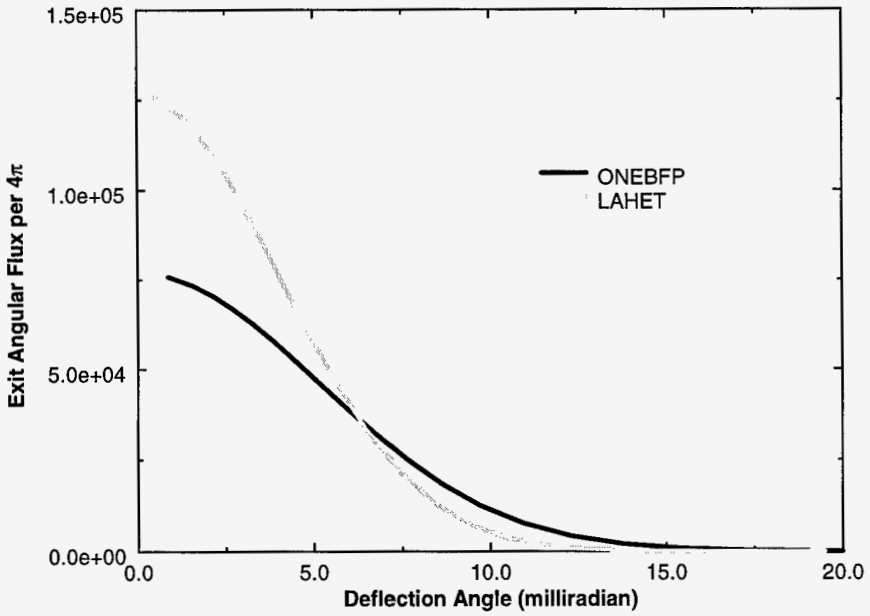

Figure 3: A similar comparison as Figure 1 except that neither code had any attenuation. Since the differences persist, it was concluded that the removal term did not cause the variation in angular dispersion.

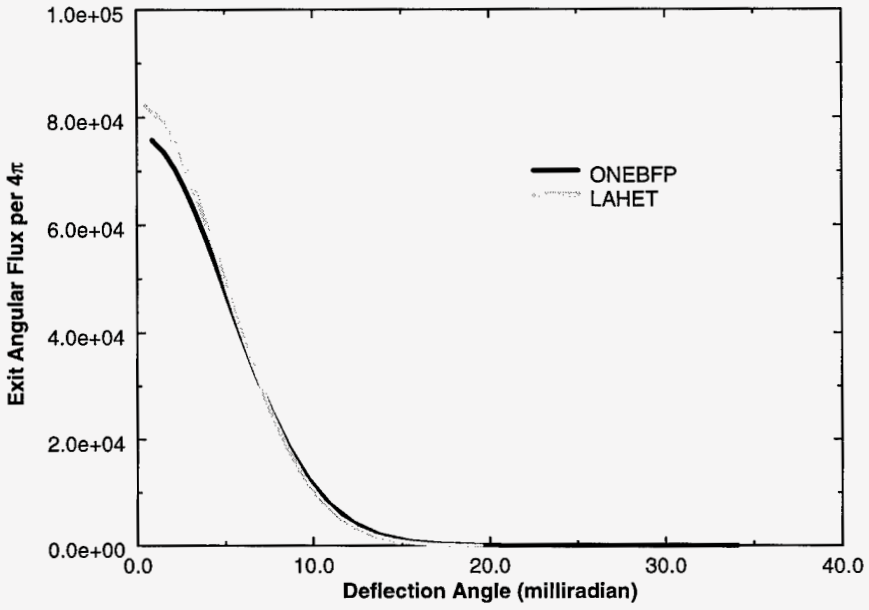

Figure 4: Comparison of ONEBFP and LAHET calculation of beam angular dispersion for 10 GeV protons normally incident on a 11.2 cm thick Copper slab. LAHET used the same momentum transfer coefficient as ONEBFP.

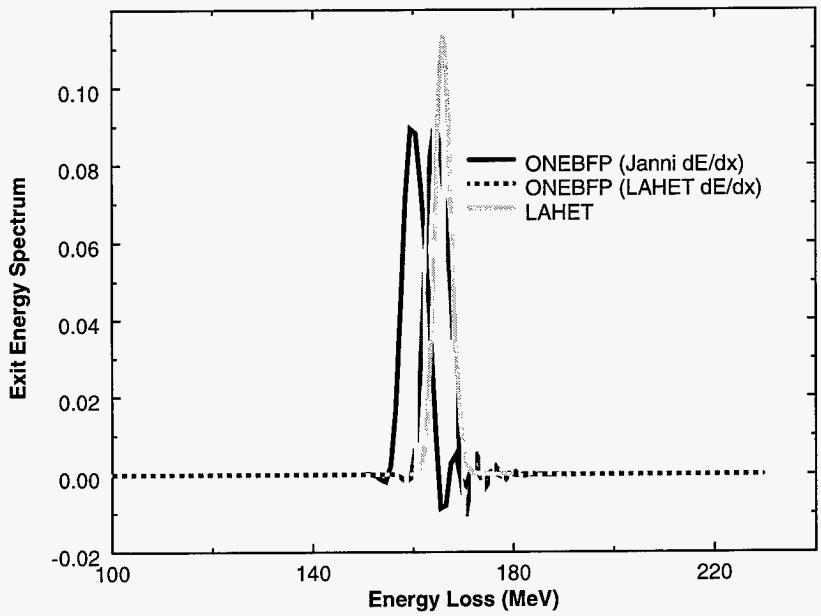

Figure 5: Comparison of ONEBFP and LAHET calculation of exit energy spectrum for protons normally incident on a 11.2 cm thick Copper slab. ONEBFP used a narrow source distribution 6 MeV wide cenetered on 10 GeV and LAHET had a monoenergetic source at 10 GeV. ONEBFP used both LAHET and Janni stopping powers (dE/dx).

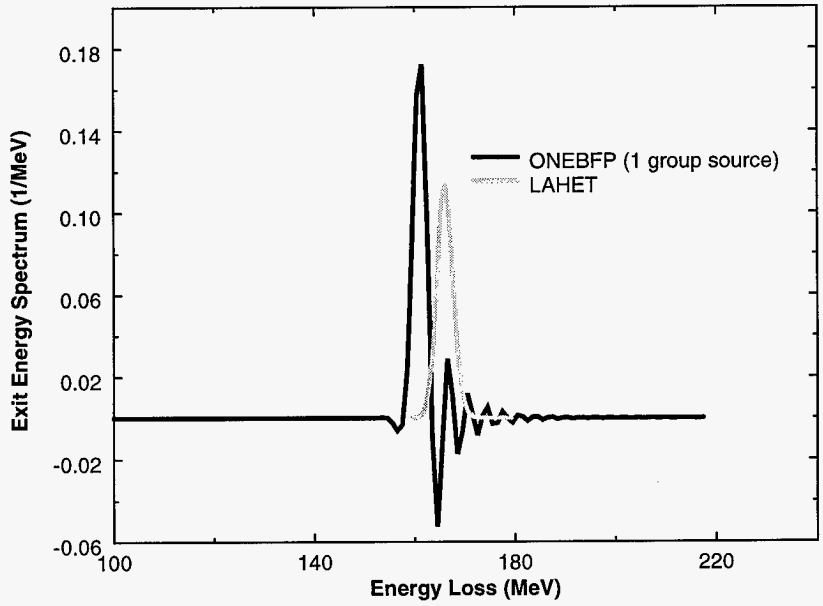

Figure 6: Comparison of ONEBFP and LAHET calculation of exit energy spectrum for protons normally incident on a 11.2 cm thick Copper slab for monoenergetic sources. The magnitude of the negative spectral values worsens for narrower sources in the ONEBFP calculation.

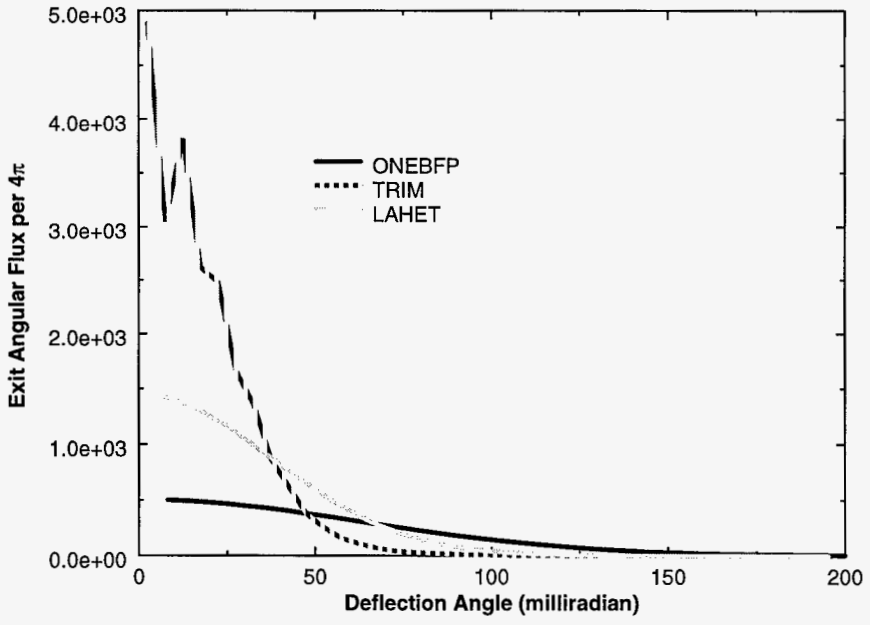

Figure 7: Comparison of ONEBFP, TRIM and LAHET calculation of beam angular dispersion for 800 MeV protons normally incident on a 11.2 cm thick Copper slab.

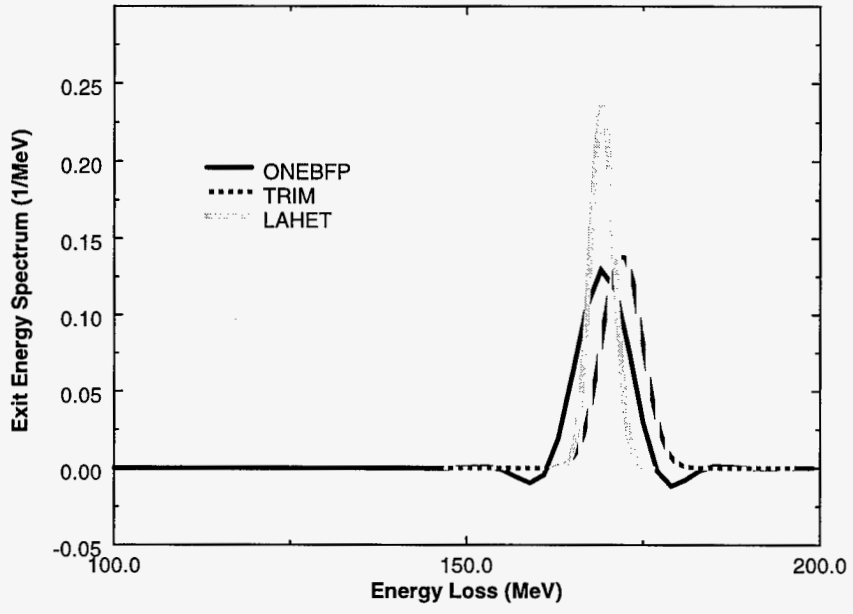

Figure 8: Comparison of ONEBFP, TRIM, and LAHET calculation of exit energy spectrum for 800 MeV protons normally incident on a 11.2 cm thick Copper slab for monoenergetic sources.

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