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Exponential Discontinuous Solution of the Multispecies Relativistic Heavy Ion Transport Equations

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Linear schemes applied to charged particle transport problems demonstrate high order accuracy but under certain conditions can also produce negative solutions. On the other hand, the recently developed nonlinear exponential discontinuous (ED) method has been shown to produce accurate strictly positive solutions, for positive sources, in neutral particle transport applications.[1] We have applied this method to the solution, in space and energy, of the multispecies transport equations for relativistic heavy ions. The solution may be useful as a treatment planning tool for the irradiation of certain cancers using heavy ions. Collisions between projectile ions and atoms in the target medium can result in ion fragments different from the original species. The solution includes these projectile fragments. The primary ion and all fragments are treated using the straight ahead approximation under which the fragments continue on with the same velocity as the original projectile.

The flux, $\psi_n(x,E)$, of an n-type particle with energy E at x is given by

$$\frac{\partial\psi_n(x,E)}{\partial x}+\sigma_n(x,E)-\frac{\partial}{\partial E}\left[S_n(E)\psi_n(x,E)\right]=Q_n(x,E) \qquad (1)$$

where $\sigma_n(x,E)$ is the absorption cross section of the n-type particle, $S_n(E)$ is the stopping power of the target medium for an n-type particle, and $Q_n(x,E)$ is the source of n-type particles due to projectile fragmentation. Energy losses are most commonly

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treated using the continuous slowing down (CSD) approximation. In the ED solution, the stopping power and cross sections are taken to be piece-wise constant in each phase space cell.

The first step in the ED solution is to form the zeroth, the first spatial (*x*), and the first energy (*E*) moments of equation (1). These moments are given by

$$\frac{1}{\Delta x_i}\left(\phi^{RA}_{n,i,g}-\phi^{RA}_{n,i-1,g}\right)+\sigma_{n,i,g}\phi^{A}_{n,i,g}-\frac{S_{n,i,g}}{\Delta E_g}\left(\phi^{BA}_{n,i,g-1}-\phi^{BA}_{n,i,g}\right)=Q^{A}_{n,i,g} \quad (2)$$

$$\frac{3}{\Delta x_i}\left(\phi^{RA}_{n,i,g}+\phi^{RA}_{n,i-1,g}-2\phi^{A}_{n,i,g}\right)+\sigma_{n,i,g}\phi^{X}_{n,i,g}-\frac{S_{n,i,g}}{\Delta E_g}\left(\phi^{BX}_{n,i,g-1}-\phi^{BX}_{n,i,g}\right)=Q^{X}_{n,i,g} \quad (3)$$

$$\frac{1}{\Delta x_1}\left(\phi^{RE}_{n,i,g}-\phi^{RE}_{n,i-1,g}\right)+\sigma_{n,i,g}\phi^{E}_{n,i,g}-\frac{3S_{n,i,g}}{\Delta E_g}\left(\phi^{BA}_{n,i,g-1}+\phi^{BA}_{n,i,g}-2\phi^{A}_{n,i,g}\right)=Q^{E}_{n,i,g} \quad (4)$$

The three moment equations have seven unknowns given by the superscripted $\phi_{n,i,g}$, all of which involve integrals of the flux $\psi_n(x,E)$. The transport parameters, which are dependent on the phase space variables, have been replaced with group constants. The $S_{n,i,g}$ are the group average stopping powers and $\sigma_{n,i,g}$ are the group average absorption cross sections. The zeroth source moment for the first generation of fragments is $Q^{A}_{n,i,g}=\phi^{A}_{p,i,g}\sigma^{f}_{p,n,i,g}$ where $\sigma^{f}_{p,n,i,g}$ is the cross section for the production of an *n*-type fragment from a *p*-type projectile in the g^{th} energy group in the i^{th} spatial cell. The first spatial and energy source moments have a similar form. The seven unknowns are reduced to three by the substitution of an exponential ansatz of the form

$$\psi_n(x,E)=a_{n,i,g}e^{\lambda_{n,i,g}P_1(x)+\eta_{n,i,g}P_1(E)} \quad (5)$$

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where $P_1(x) = \frac{2}{\Delta x_i}(x - x_i)$ and $P_1(E) = \frac{2}{\Delta E_g}(E - E_g)$. After this substitution, the three unknowns, $a_{n,i,g}$, $\lambda_{n,i,g}$, and $\eta_{n,i,g}$, are determined by a marching Newton-Raphson iteration of the resulting moment equations in successive phase space cells.

This algorithm and a linear discontinuous (LD) solution for equation (1) were written into the ELDRHIT (**E**xponential and **L**inear **D**iscontinuous **R**elativistic **H**eavy **I**on **T**ransport) code to investigate the ED technique as a method of solution for equation (1) and to compare this solution with that of the LD scheme, keeping in mind that the LD solution is the thin cell limit of the ED solution. Separate codes were developed for the absorption and fragmentation cross sections. Group constant absorption cross sections were based on the parameterization of Tripathi *et al* [2], while group constant fragmentation cross sections were calculated using an adaptation of the NUCFRG code of Wilson *et al.*[3] Calculated results are compared with the experimental results of Schimmerling *et al.*[4]

The method was applied to a monoenergetic beam of fully ionized 636.28 MeV per nucleon neon-20 impinging upon a water slab. These conditions correspond to the experimental conditions of Reference 4. The range of such particles in water is approximately 34 cm. The calculations of $a_{n,i,g}$, $\lambda_{n,i,g}$, and $\eta_{n,i,g}$ were individually converged to a relative error of 10^{-8}.

Figure 1 shows a dose comparison of ED and LD calculations for two different phase space meshes: a 50 group, 50 cell mesh (50/50) and a 100-group, 100-cell mesh (100/100). Neither method accurately captures the Bragg peak and both methods show a significant amount of numerical straggle beyond the actual range. The LD solutions, while indicating slight improvement over comparable ED solutions, do so at the expense of negative doses at the end of the target material. These results were cause for concern since the primary neon solution is required to calculate the fragment sources.

To satisfy the requirement for an accurate fragment source distribution, an exact solution for the primary neon particle was used and ED and LD solutions were used for the fragments. This approach is analogous to the first scattered distributed source (FSDS) technique. Calculated total average linear energy transfer (LET) values for all fragments considered in Reference 4 were compared with the experimental results of Schimmerling *et al.* In keeping with Schimmerling's practice, the total average LET was normalized to the neon LET at the entrance to the experimental water column. This approach, using the ED method for the fragments, demonstrates excellent agreement with experiment, as shown in Figure 2.

The basic conclusion from this work is that using the exact solution for the primary particle coupled with an ED solution for the fragments provides an accurate solution for all particle species.

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Figure 1. ED/LD Primary Neon Dose Comparison

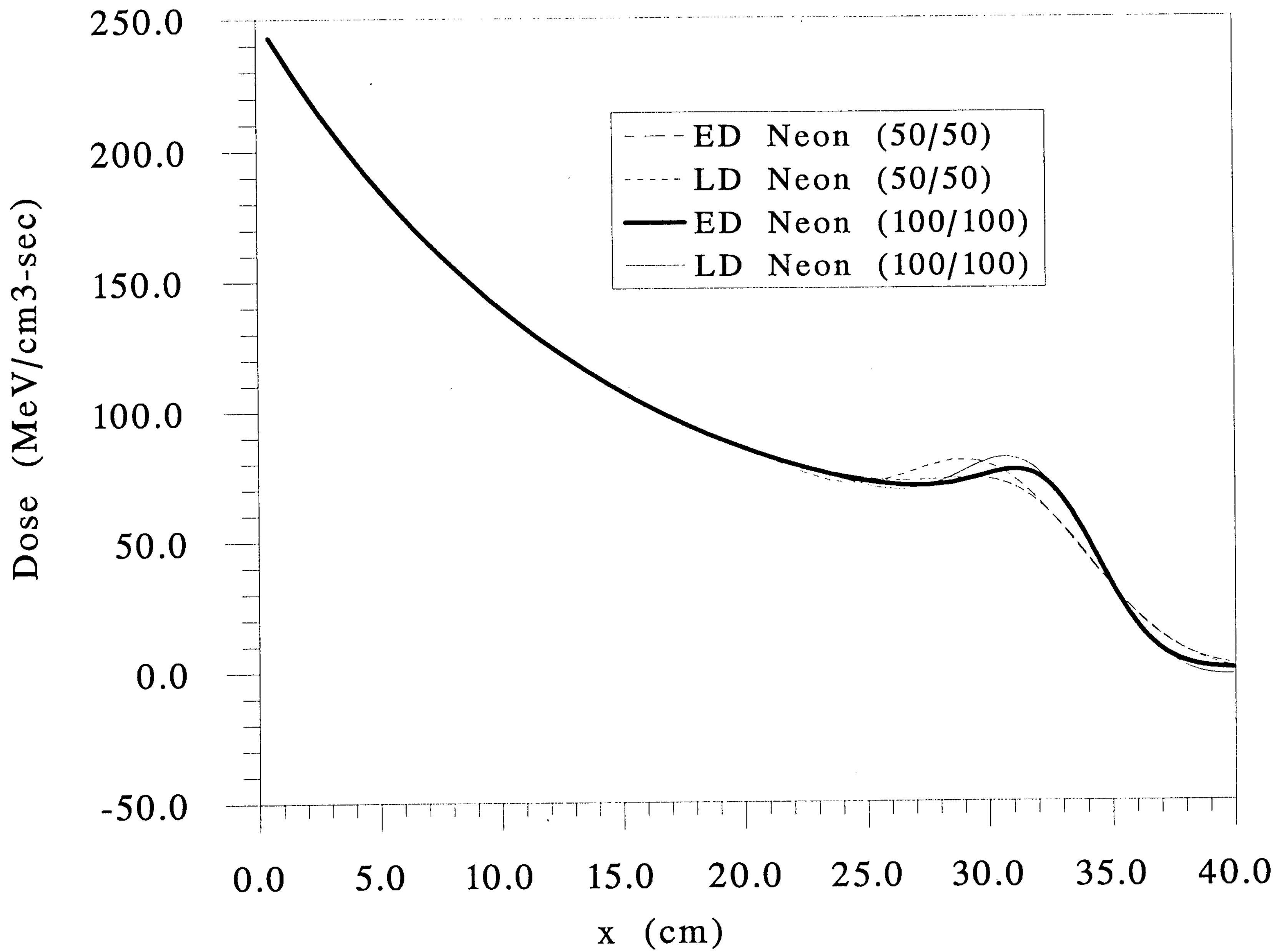
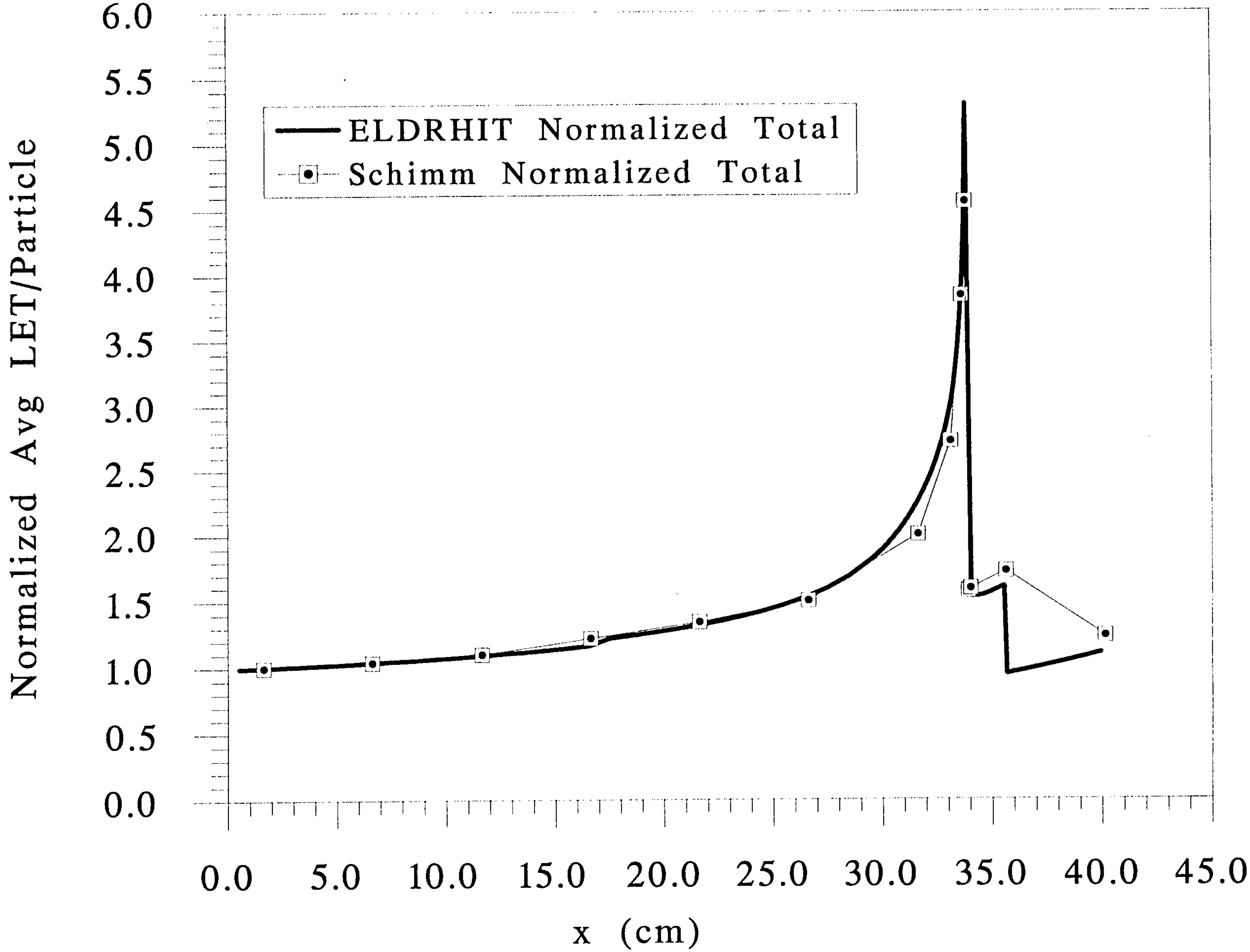


Figure 2. ELDRHIT - Schimmerling Total Avg LET/Particle Comparison



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