Modeling ion beam energy deposition distributions

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The Field Precision codes **Trak** and **OmniTrak** model the generation and transport of ion beams as well as electron beams. For electrons, results may be ported to the Monte Carlo code **GamBet** for detailed models of interactions with matter. The energy deposited through multiple processes can be used to analyze dose distributions and thermal energy. In turn, the information can be transferred to the codes **TDiff** and **HeatWave** to model target heating. Following increasing interest in proton beams for radiation treatments, we are building a companion code to **GamBet** to handle light ion interactions with matter. The following factors make it relatively easy to extend our existing codes to make calculations of dose deposition and heating by high-energy ions in matter:

- In contrast to the complex interactions of electrons (bremsstrahlung, Compton scattering,...), ions slow primarily by collisions with atomic electrons.
- Because of the mass disparity, the interactions do not generate high energy secondary electrons or photons.
- Nuclear reactions account for only a small fraction of energy loss.
- Ions move in almost straight lines as they slow.

Our first step is to build a database appropriate for inclusion in the finite-element framework developed for **GamBet**. It will be based on **SRIM**[1], a widely-used tool for ion energy exchange with matter. We can use the code to illustrate the validity of the listed factors. A **SRIM** calculation with 250 MeV protons (typical of proton therapy devices) in a generic tissue model yields a range of 358.61 ± 14.94 mm. The width of the beam at the end of the range is 8.24 mm, implying that a straight line projection of the incident ion trajectory is accurate to $\pm 1.3^{o}$. The energy loss via nuclear processes averaged over the trajectory is only 0.07% of the energy loss to electrons. The implication is that given a distribution of ions incident on a target from a **Trak** or **OmniTrak** calculation, a detailed shower calculation is not necessary to find dose and deposited energy. Accurate estimates can be determined by approximately straight-line projections of the model particle orbit combined with stopping power data from **SRIM**. This report describes the program **IonDepo**, a utility to transform **SRIM** data to a form appropriate for finite-element analyses.

[1] Stopping and Range of Ions in Matter, http://www.srim.org.

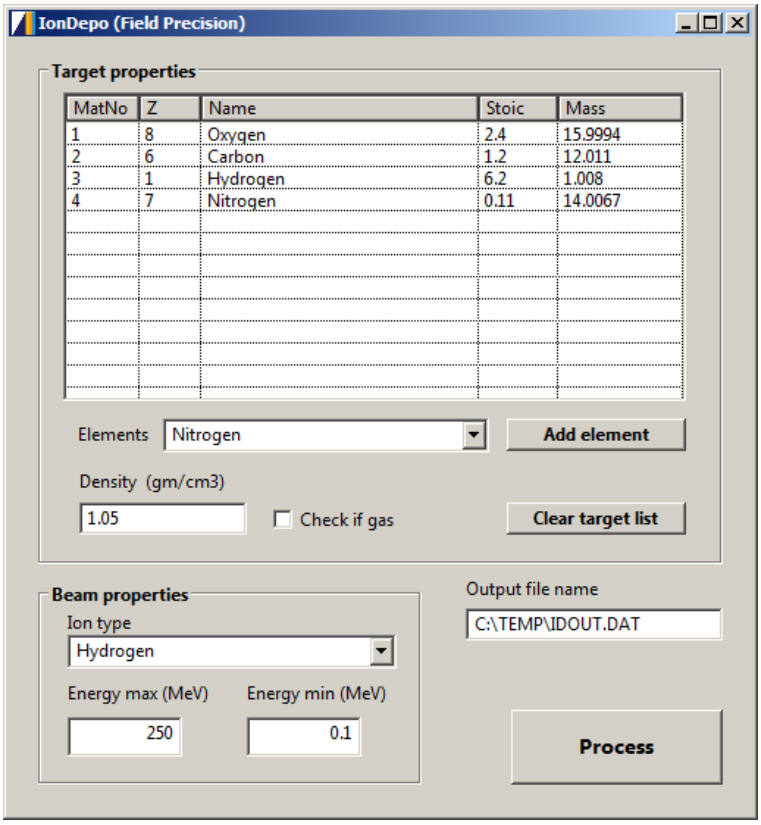

Figure 1: **IonDepo** interface, settings for an ion therapy dose calculation.

The command-line version of **SRIM** (`SRModule.exe`) generates a text table of the initial stopping power (electronic and nuclear) and range as a function of incident ion energy for specified materials. Dose and thermal calculations require data in a different format, the relative energy loss for a model ion as a function of depth in the material. The program **IonDepo** has two functions:

- Provide an interactive interface to `SRModule.exe`.
- Convert the output to a form suitable for finite-element calculations with standard units.

Figure 1 shows the program interface. The target composition is defined by a list of elements along with their stoichiometric contributions (the relative number of atoms). Up to 12 elements may be chosen from a popup menu. The choice automatically supplies the value of Z and the atomic mass (in amu). The `Stoic` column is editable. This quantity as well as the compound density are user supplied. The incident ion and its required parameters are also supplied from a popup menu. The user sets the incident and final

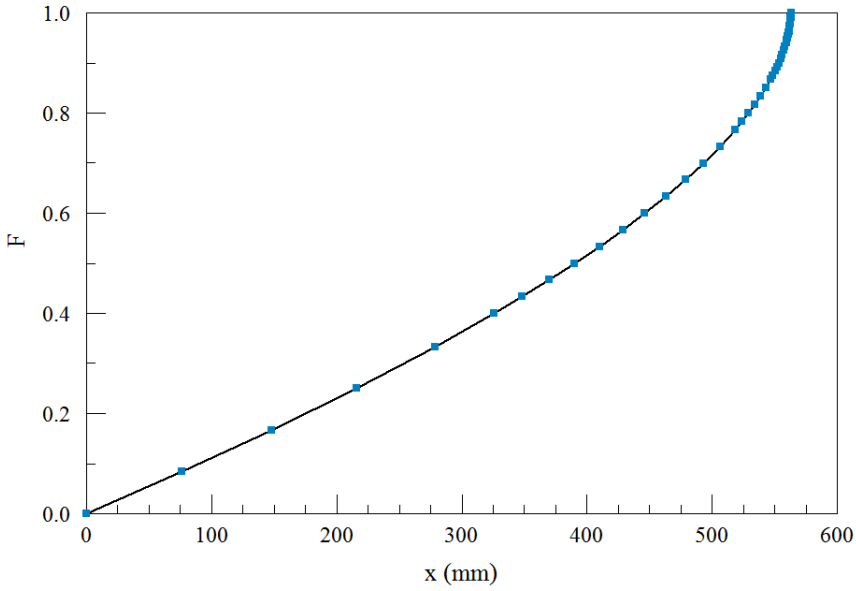

Figure 2: Table entries for $F(z)$, the fraction energy loss as a function of depth (300 MeV protons in water).

energies and the path and name of the output text data file. When setup is complete, the calculation proceeds automatically in response to the `Process` button.

SRIM output consists of a list of injection energies (E_i) and values of the stopping power at the injection point ($dEdz_i$). For deposited energy calculations, we need a single particle history: energy and stopping power as a function of depth in the material. The energy and stopping power can be expressed as a function of depth using the following difference relationship:

$$z_{i+1} = z_i + \frac{2(E_i - E_{i+1})}{dEdz_1 + dEdz_{i+1}}. \tag{1}$$

where $z_0 = 0.0$. **IonDepo** runs **SRIM** with the specified input parameters and creates a table of z_i, $E(z_i)$, $dEdz(z_i)$ and other quantities from the output file:

```
IonDepo (Field Precision LLC)
  Monday, January 08, 2024  11:00:41 AM

Incident ion properties
  Name: Hydrogen
  Z: 1
  Mass: 1.008 (amu)
  Energy: 200.000 (MeV)
  Range: 256.288 (mm)
Target composition
  Solid
  1:  Hydrogen (2.0)
  2:  Oxygen (1.0)
```

z(mm)	E(Mev)	dE/dz(MeV/mm)	SigmaZ(mm)	SigmaR(mm)	F
0.0000	200.0000	0.4540	9.9700E+0	6.1700E+0	0.0000
42.5411	180.0000	0.4863	7.8800E+0	5.1900E+0	0.1000
62.7106	170.0000	0.5053	7.3100E+0	4.7200E+0	0.1500
82.0939	160.0000	0.5265	6.7400E+0	4.2700E+0	0.2000
100.6650	150.0000	0.5504	6.1800E+0	3.8300E+0	0.2500
118.3944	140.0000	0.5776	5.6200E+0	3.4100E+0	0.3000
135.2507	130.0000	0.6089	5.0700E+0	3.0100E+0	0.3500
151.2030	120.0000	0.6449	4.5100E+0	2.6200E+0	0.4000
166.2170	110.0000	0.6872	3.9600E+0	2.2600E+0	0.4500
180.2557	100.0000	0.7374	3.4000E+0	1.9200E+0	0.5000

```
 ...
```

The quantity σ_z is the longitudinal straggling, the variation in range resulting from statistical processes. The quantity σ_r is the lateral spread, the deviation from straight line motion. Finally, F is the fraction of the incident energy lost – it varies from 0.0 to 1.0. The values of z_i converge at the range corresponding to the injection energy. For the example of Fig. 1, the transform of Eq. 1 gives a range of 376.62 mm, within 0.02% of the listed **SRIM** value of 376.55 mm. Figure 2 shows the variation of F and the convergence of table entries for 300 MeV protons in water.

Field Precision has tested code components to build an ion dose program:

- The programs **Trak**, **OmniTrak** or **GenDist** can create generalized input distributions with large numbers of ions.
- **IonDepo** will be applied to create a database of standard files for light ion interactions in an assortment of materials (*e.g.*, brain tissue, bones, muscle tissue,...). Program users can apply **IonDepo** along with their copy of **SRIM** to add material files for specialized applications.
- The existing programs (**Mesh**, **Geometer** and **MetaMesh**) create 2D/3D conformal meshes with shaped regions to represent different materials.
- **OmniTrak**, **Trak** and **GamBet** have routines to track large numbers of model particles through conformal meshes. Available routines will be adapted for operations such as identification of the element at ion

positions and determination of the entrance and exit locations between tissue regions. As in **GamBet**, ion energy deposition will be resolved on an element scale.

- Procedures exist to transfer element-based energy or power profiles directly to **TDiff** or **HeatWave** for thermal calculations.

In **GamBet**, model electrons may follow complex shower histories. Each shower could include the generation of secondary electrons or photons which have their own set of interactions. Model electrons with the same entrance parameters could have entirely different outcomes; therefore, a large set of calculations is required for statistical accuracy. In contrast, the history of a model ion is almost deterministic with no high-energy secondary particles. The spatial step size for tracking a trajectory is based on the range, a known value with statistical variations given by σ_z. The ion trajectory is a straight line with a small lateral random walk determined by σ_r. The implication is that an ion dose code would run quite fast, opening the possibility of real time applications.