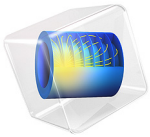

Ion Range Benchmark

Introduction

When ions strike the surface of a solid material at extremely high energy, they may penetrate a significant distance into the target material or even pass through it. The exchange of energy between the incident ions and atoms within the target material forms the basis of a class of interactions known broadly as Single Event Effects (SEEs).

In harsh radiation environments, SEEs can cause a variety of undesirable phenomena in sensitive electronic equipment, ranging from soft errors such as bit flips to hard/permanent problems such as single event latchup or burnout. For this reason, understanding of SEEs is vital when designing electronic devices for harsh radiation environments such as outer space.

This example demonstrates an approach to modeling the interaction of energetic ions with a target material using dedicated features in the Charged Particle Tracing interface. These features are used to compute the average distance traversed by protons in silicon, which is then compared to empirical data over a range of initial energy values.

Model Definition

The Charged Particle Tracing interface includes dedicated nodes for modeling the interaction of ions with solid materials. The **Particle-Matter Interaction** node accounts for the energy loss and scattering of incident ions in the solid material by supporting dedicated subnodes for the following types of interactions:

- The **Ionization Loss** subnode treats the interaction between incident ions and electrons in the target material as a continuous force that acts opposite the direction of the particle's motion.
- The **Nuclear Stopping** subnode treats the interaction between incident ions and nuclei in the target material as a discrete force that both slows the ion and deflects it by a random angle with a certain probability.

The validity of this approach is confirmed by this simple benchmark model. Protons are released into a block of silicon with a specified initial energy. They are then subjected to the deterministic ionization losses and stochastic nuclear interactions until their average velocity becomes negligibly small. By using an **Auxiliary Dependent Variable** to compute the path length of each ion in the target, the average range of the ions is computed. This average range is then compared to the tabulated range under the Continuous Slowing Down Approximation (CSDA range) as given by Ref. 1. Under the CSDA, the ions are assumed to decelerate so that rate of energy loss is the same at every point along the ion's trajectory:

$$R_{\mathrm{CSDA}} = \int_{E_f}^{E_i} \frac{1}{S(E)} dE$$

where E_i and E_f are the initial and final energy of the ion, respectively, and $S(E)$ is the total stopping power as a function of the ion energy.

An alternative means of reporting the ion range is the projected range, which indicates the approximate penetration depth into the target material. The projected range is computed by first projecting the ion velocity onto the initial direction of propagation.

Results and Discussion

The particle trajectories are computed for initial energy values ranging from 1 keV to 100 MeV. In general, as the energy increases, the particles move in more linear trajectories as their deceleration is dominated by ionization loss. At lower initial energy values, the ion trajectories are dominated by nuclear interactions and the ions tend to move in random directions. A typical plot of the ion trajectories is shown in Figure 1.

The average ion range is reported in Figure 2 and compared to published values from Ref. 1. Both the CSDA range and the projected range are shown. As the initial ion energy increases, the agreement between the CSDA range and computed range improves because the decrease in ion energy is dominated by ionization losses, which cause the ions to decelerate continuously over time. The agreement between the CSDA range and the projected range improves as well because the ionization losses do not cause any change in the direction of ion propagation.

At lower initial energy, the CSDA range and projected range differ significantly because the ion trajectories are dominated by nuclear stopping, which causes their energy to change discontinuously and also deflects them from their initial direction of propagation. The computed path lengths then show closer agreement to the projected range than the CSDA range.

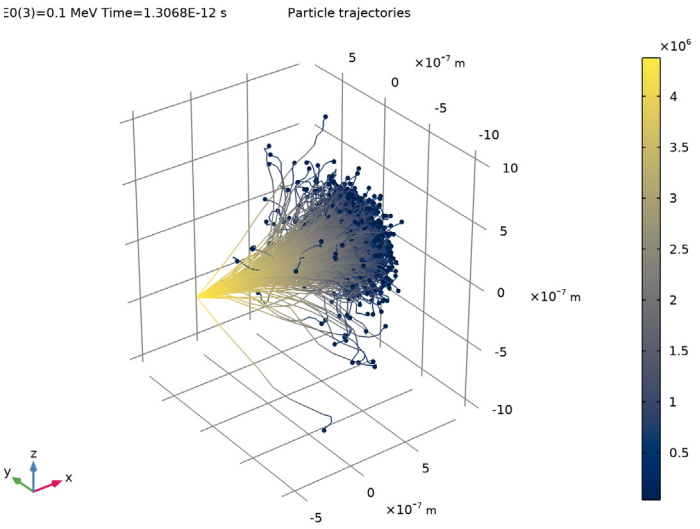

Figure 1: Trajectories of 0.1 MeV protons in silicon. The changes in direction are due to collisions with target nuclei. The continuous decrease in energy is from ionization loss.

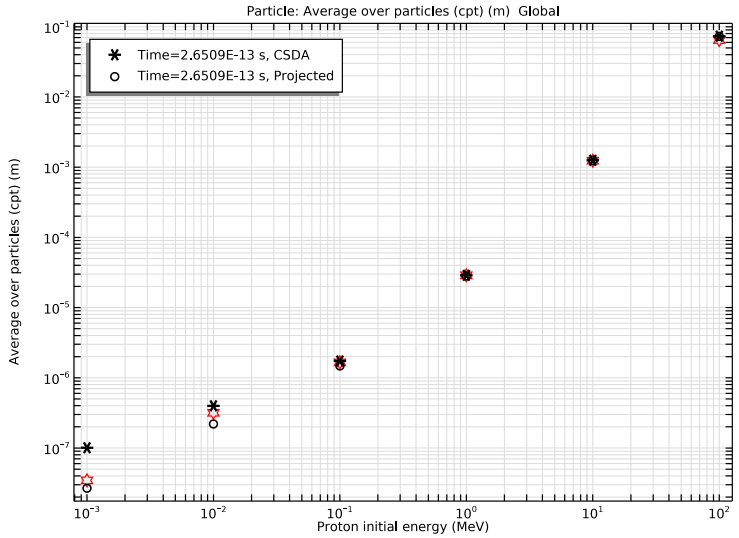

Figure 2: Comparison of the average path length of the computed ion trajectories to the published values of the ion range. Both the CSDA range and projected range are reported.

Reference

1. NIST Stopping-Power and Range Tables for Electrons, Protons, and Helium Ions, http://www.nist.gov/pml/data/star/index.cfm

Application Library path: `Particle_Tracing_Module/Charged_Particle_Tracing/ion_range_benchmark`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **AC/DC>Particle Tracing>Charged Particle Tracing (cpt)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

Load the model's parameters.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `ion_range_benchmark_parameters.txt`.

DEFINITIONS

Load data for the CSDA range of protons in silicon.

Interpolation 1 (int1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `ion_range_benchmark_ranges.txt`.

6 In the **Number of arguments** text field, type `1`.

7 Click **Import**.

8 Find the **Functions** subsection. In the table, enter the following settings:

Function name	Position in file
CSDA	1

9 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
Column 1	MeV

10 In the **Function** table, enter the following settings:

Function	Unit
CSDA	g/cm^2

Load data for the projected range of protons in silicon.

Interpolation 2 (int2)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `ion_range_benchmark_ranges.txt`.

6 In the **Number of arguments** text field, type `1`.

7 Find the **Functions** subsection. In the table, enter the following settings:

Function name	Position in file
Proj	2

8 Click **Import**.

9 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
Column 1	MeV

10 In the **Function** table, enter the following settings:

Function	Unit
Proj	g/cm^2

Create a block of silicon of length L centered at the origin. The value of L will be varied as a function of the particles' initial energy E_0 -- see the Parameters list.

GEOMETRY 1

Block 1 (blk1)

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type L.

4 In the **Depth** text field, type L.

5 In the **Height** text field, type L.

6 Locate the **Position** section. From the **Base** list, choose **Center**.

7 Click **Build All Objects**.

At the maximum simulated energy of 100 MeV, the proton velocity is comparable in magnitude to the speed of light, so select the **Relativistic correction** option.

CHARGED PARTICLE TRACING (CPT)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Charged Particle Tracing (cpt)**.

2 In the **Settings** window for **Charged Particle Tracing**, locate the **Particle Release and Propagation** section.

3 Select the **Relativistic correction** check box.

Particle-Matter Interactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Particle-Matter Interactions**.

2 Select Domain 1 only.

Ionization Loss 1

In the **Physics** toolbar, click **Attributes** and choose **Ionization Loss**.

Particle-Matter Interactions 1

In the **Model Builder** window, click **Particle-Matter Interactions 1**.

Nuclear Stopping 1

In the **Physics** toolbar, click **Attributes** and choose **Nuclear Stopping**.

Enter the particles' rest mass and charge number using the variables defined in the model parameters.

Particle Properties 1

1. In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Particle Properties 1**.
2. In the **Settings** window for **Particle Properties**, locate the **Particle Species** section.
3. From the **Particle species** list, choose **Proton**.

Create a release of 1001 particles of initial energy E_0 directed in the positive x direction. The particles will be released at $x = -L/4$ in order to observe backscattered ions at low initial energies.

Release from Grid 1

1. In the **Physics** toolbar, click **Global** and choose **Release from Grid**.
2. In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.
3. In the $q_{x,0}$ text field, type `-L/4`.
4. Click **Y Range**.
5. In the **Range** dialog box, choose **Number of values** from the **Entry method** list.
6. In the **Start** text field, type `-L/1e3`.
7. In the **Stop** text field, type `L/1e3`.
8. In the **Number of values** text field, type `1001`.
9. Click **Replace**.
10. In the **Settings** window for **Release from Grid**, locate the **Initial Velocity** section.
11. From the **Initial velocity** list, choose **Kinetic energy and direction**.
12. In the E_0 text field, type `E0`.

Add an auxiliary variable `rp` to the model. The auxiliary variable will be used to compute the total length of the particle trajectory.

Auxiliary Dependent Variable 1

1 In the **Physics** toolbar, click **Global** and choose **Auxiliary Dependent Variable**.

2 In the **Settings** window for **Auxiliary Dependent Variable**, locate the **Auxiliary Dependent Variable** section.

3 In the R text field, type `1`.

4 From the **Integrate** list, choose **Along particle trajectory**.

5 Locate the **Units** section. Click **Select Quantity**.

6 In the **Physical Quantity** dialog box, type `length` in the text field.

7 Click **Filter**.

8 In the tree, select **General>Length (m)**.

9 Click **OK**.

Enter values for the material properties of silicon.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	`rhoSi`	kg/m³	Basic

STUDY 1

Add a **Parametric Sweep** over the initial energy with a minimum value of 1 keV and a maximum value of 100 MeV.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E0 (Proton initial energy)		`MeV`

5 Click **Range**.

6 In the **Range** dialog box, choose **exp10(x) – Exponential function (base 10)** from the **Function to apply to all values** list.

7 In the **Start** text field, type `-3`.

8 In the **Step** text field, type `1`.

9 In the **Stop** text field, type `2`.

10 Click **Replace**.

Step 1: Time Dependent

1 In the **Model Builder** window, click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,1/20,1)*tmax`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

Modify the default solver sequence to set a manual time step size. It is important that the time step is sufficiently small to resolve individual collisions when the ion trajectories are dominated by nuclear stopping.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

4 From the **Steps taken by solver** list, choose **Manual**.

5 In the **Time step** text field, type `tmax/1e3`.

6 In the **Study** toolbar, click **Compute**.

RESULTS

Particle Trajectories (cpt)

1 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

2 Clear the **Plot dataset edges** check box.

3 Locate the **Data** section. From the **Parameter value (E0 (MeV))** list, choose **0.1**.

Particle Trajectories 1

1 In the **Model Builder** window, expand the **Particle Trajectories (cpt)** node, then click **Particle Trajectories 1**.

2 In the **Settings** window for **Particle Trajectories**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Type** list, choose **Line**.

Color Expression 1

1 In the **Model Builder** window, expand the **Particle Trajectories 1** node, then click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **Cividis**.

4 In the **Particle Trajectories (cpt)** toolbar, click **Plot**.

5 Click the **Go to Default View** button in the **Graphics** toolbar. Compare the resulting plot to Figure 1.

Stopping Distance

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Stopping Distance` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Particle 1**.

4 From the **Time selection** list, choose **Last**.

5 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Particle 1

1 In the **Stopping Distance** toolbar, click **More Plots** and choose **Particle**.

2 In the **Settings** window for **Particle**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `cpt.ave(rp)`.

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Outer solutions**.

5 From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `E0`.

7 From the **Unit** list, choose **MeV**.

8 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

9 From the **Color** list, choose **Red**.

10 In the **Width** text field, type `2`.

11 Find the **Line markers** subsection. From the **Marker** list, choose **Star**.

12 From the **Positioning** list, choose **In data points**.

Global 1

1 In the **Model Builder** window, right-click **Stopping Distance** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`CSDA(E0)/rhoSi`	`m`	`CSDA`
`Proj(E0)/rhoSi`	`m`	`Projected`

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Outer solutions**.

5 From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `E0`.

7 From the **Unit** list, choose **MeV**.

8 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

9 From the **Color** list, choose **Black**.

10 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

11 From the **Positioning** list, choose **In data points**.

12 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

13 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

14 In the **Stopping Distance** toolbar, click  **Plot**. Compare the resulting plot to Figure 2.