Calculation of nuclear stopping power of an ion

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Contents

1 Abstruct

This project investigates the nuclear stopping power of ions penetrating matter using two models: the Ziegler, Biersack, Littmark (ZBL) screened Coulomb potential and a universal empirical formula. The stopping power, defined as the energy loss per unit path length of an ion, was computed numerically for two ion-target combinations: hydrogen (H) in silicon (Si) and silicon (Si) in gold (Au). The implementation relied on numerical integration (Gauss-Legendre quadrature) and root-finding (bisection method) to solve the scattering integrals. Results were compared between the ZBL and universal models, proving good agreement at intermediate energies but deviations at low and high energies due to approximations in the universal formula. This study demonstrates the effectiveness of numerical methods in simulating ion-matter interactions while highlighting limitations in empirical models.

2 Introduction

When an energetic ion penetrates a material, it loses energy through collisions with electrons and nuclei. Stopping power is interpreted as the rate at which a material absorbs the kinetic energy of a charged particle [2]. In this problem, we only calculated the nuclear stopping power of two different collision types, not the electronic stopping power.

The nuclear stopping power quantifies the energy loss due to elastic collisions with target atoms. Understanding this phenomenon is crucial in fields such as materials science, radiation protection, and semiconductor device fabrication.

This project computes the nuclear stopping power using:

- The ZBL model, which employs a screened Coulomb potential to describe ion-atom interactions.
- A universal stopping power formula, derived from empirical fits to numerous ion-target combinations.

The goal is to compare these models numerically and assess their accuracy across a wide energy range (10 eV – 5 MeV).

3 Methods

3.1 ZBL model

For calculating the ZBL model, we need to solve the equation for the nuclear stopping power at a certain energy of the projectile in the laboratory coordinate system, Elab:

$$S_n(E_{\text{lab}}) = 2\pi\gamma E_{\text{lab}} \int_0^{b_{\max}} \sin^2\left(\frac{\Theta(b, E_{\text{com}})}{2}\right) b\, db \tag{1}$$

The reduced mass γ can be calculated from the formula below.

$$\gamma = \frac{4M_1M_2}{(M_1+M_2)^2} \tag{2}$$

Next, we need to get the integral $\int_0^{b_{\max}} \sin^2\left(\frac{\Theta(b,E_{\text{com}})}{2}\right) b\, db$ value between b and b_{max}. We get the integral value by the

$$\Theta = \pi - 4b\int_0^1 F(u)\, du \tag{3}$$

$$F(u) = \left[b^2(2-u^2) + \frac{r_{\min}^2}{u^2 E_{\text{com}}}\left(V(r_{\min}) - V\left(\frac{r_{\min}}{1-u^2}\right)\right)\right]^{-1/2} \tag{4}$$

$$r = \frac{r_{\min}}{1-u^2}, \quad dr = \frac{2r_{\min}u\, du}{(1-u^2)^2} \tag{5}$$

And lastly, to substitute the value of potential V, the following equations are used,

$$V(r) = \frac{Z_1Z_2e^2}{4\pi\varepsilon_0 r} \cdot \Phi\left(\frac{r}{a_u}\right) \tag{6}$$

$$a_u = \frac{0.46848\,\text{Å}}{Z_1^{0.23} + Z_2^{0.23}} \tag{7}$$

$$\Phi(x) = \sum_{i=1}^{4} \alpha_i e^{-\beta_i x} \tag{8}$$

And we search for the value of r_{min} by using the

$$g(r) = \sqrt{1 - \left(\frac{b}{r}\right)^2 - \frac{V(r)}{E_{\text{com}}}} \tag{9}$$

equation at $g(r_{min}) = 0$.

- For $H \rightarrow Si$ system, the M_1 is 1.00784 M_2 is 28.0855 and $Z1 = 1, Z2 = 14$;
- For $Si \rightarrow Au$ system, the M_1 is 28.0855 M_2 is 196.96657 and $Z1 = 14, Z2 = 79$;

The E_{lab} range is from 10 eV to 5 MeV.

3.2 Universal model

The universal model is determined by taking the empirical coefficients from multiple datasets. The formula used here can be written as,

$$S_n(E_{\text{com}}) = \frac{8.462 \times 10^{-15} Z_1 Z_2 M_1}{(M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})} \cdot s_n(\epsilon) \tag{10}$$

$$s_n(\epsilon) = \begin{cases} \frac{\ln(1+1.138\epsilon)}{2(\epsilon + 0.01321\epsilon^{0.21226} + 0.19593\epsilon^{0.5})}, & \epsilon \leq 30 \\ \\ \frac{\ln \epsilon}{2\epsilon}, & \epsilon > 30 \end{cases} \tag{11}$$

$$\epsilon = \frac{32.53 E_{\text{com}}}{Z_1 Z_2 (Z_1^{0.23} + Z_2^{0.23})} \tag{12}$$

Note that this formula is an empirical fit. So, there is a good chance of deviation from the numerical solution.

3.3 Numerical Techniques and Unit handling

For the equations mentioned above, the bisection method is used as a root-finding method for the distance of closest approach r_{min}. The scattering angle integral and the stopping power integral are computed using Gauss-Legendre quadrature. Final stopping power converted to $eV/(atoms/cm^2)$. These numerical methods are adapted from the lecture [1].

Here, the unit used in the nuclear stopping power calculation is $ev/atoms/angstrom^2$. After the main calculation, it converts to $ev/atoms/cm^2$.

4 Implementation

The numerical implementation was developed in Python and organized into a modular script that calculates nuclear stopping power using the Ziegler–Biersack–Littmark (ZBL) and Universal models. The script handles two ion-target systems: **hydrogen in silicon (H → Si)** and **silicon in gold (Si → Au)**. Calculations are performed over a user-defined energy range from 10 eV to 5 MeV, and the results are saved for comparison and visualization.

Screening Potential and Energy Terms

The code begins by defining physical constants and the ZBL screening function $\Phi(x)$, implemented in the `screening_function(x)` routine. The inter-nuclear potential $V(r)$ is computed by the function `potential(r, Z1, Z2, a_u)`, which evaluates the screened Coulomb interaction using the atomic numbers and the ZBL screening length.

Closest Approach and Scattering Angle

The function `g_tilde(r, ...)` defines the root-finding equation $g(r) = 0$ for locating the distance of closest approach $r_{\min}$, given an impact parameter b. This is solved using the bisection method in `find_r_min()`. The result is passed to `scattering_angle()`, which computes the deflection angle $\Theta(b)$ via Gauss-Legendre quadrature. The integral is evaluated using a transformation over the variable $u \in [0, 1]$.

ZBL Nuclear Stopping Power

The function `nuclear_stopping_ZBL()` performs the outer integral over impact parameters. It implements equation 1. Both the Θ and b integrals are evaluated numerically using Gauss-Legendre quadrature. The final result is the nuclear stopping power in units of eV/(atoms/cm^2).

Universal Model Calculation

The Universal model is implemented in `nuclear_stopping_universal()`, which uses a closed-form expression based on empirical fits to ZBL results. It calculates the reduced energy ϵ and the corresponding reduced stopping cross-section $s_n(\epsilon)$ using a piecewise-defined function. No integration is required, making this method computationally efficient for large energy grids.

Execution Flow and Output

In the `main` block, the program:

- Defines the energy grid using a logarithmic scale over 30 points,
- Computes the nuclear stopping power for both models for H $\rightarrow$ Si and Si $\rightarrow$ Au,
- Stores the results in `pandas` DataFrames and writes them to CSV files:
  - `H_Si_stopping_power.csv`
  - `Si_Au_stopping_power.csv`
- Generates a log-log plot comparing the models and saves it as `Nuclear_Stopping_Power_Comparison.png`,
- Computes and prints the maximum relative difference between the ZBL and Universal model predictions for both ion-target systems.

In the figure 1, there is a flow diagram to describe the flow of the function of the code.

5 Using the code

The required commands are provided in the `command.sh`. **However, it may take a lot of time to complete the convergence test. The `nuclear_stopping.py` script takes around 15 minutes to complete. However, if you want to check the validity of the code, change the value of `E_lab, order,b_max_factor`.**

The `convergence_test.py` will run the convergence test and save output to the run folder as `convergence_result.csv`. The `plot_convergence.py` will plot the graphs for getting the convergence values of order and `b_max`

The main function that runs the ZBL and Universal calculation is `nuclear_stopping.py`. The running for this function is a straightforward command `python3 nuclear_stopping.py`. This will output the nuclear stopping powers of $H \rightarrow Si$ and $Si \rightarrow Au$, and a graph in the run folder in the .csv format. Lastly, `plot_relative_error.py` will plot the relative error in the run folder.

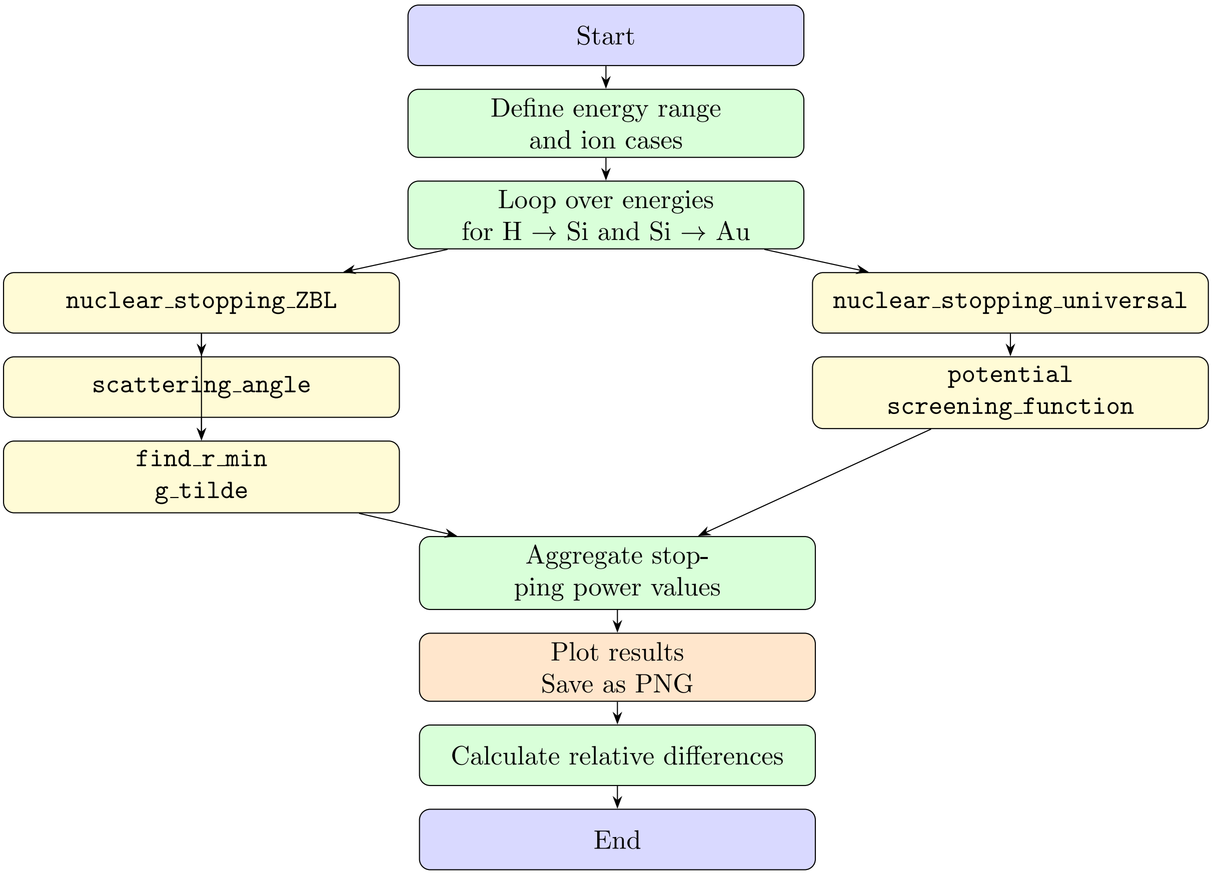


Figure 1: Figure: Function flow diagram

6 Results and Discussion

6.1 Convergence test

One of the main problems in solving this assignment is to achieve the desired accuracy. To scan all the energy values and vary order and b_{max} value, is a huge time consuming task. In the initial test, it was observed that the highest and the lowest energy values mostly deviate from the universal model. If the minimum and maximum energy values stay stable, the internal points should also stay stable. So, two points in $E_{lab} \rightarrow (10, 5000000)ev$ are chosen for getting a rough estimation of the order and $b_{max} * a_u$ value for both $H \rightarrow Si$ and $Si \rightarrow Au$ cases.

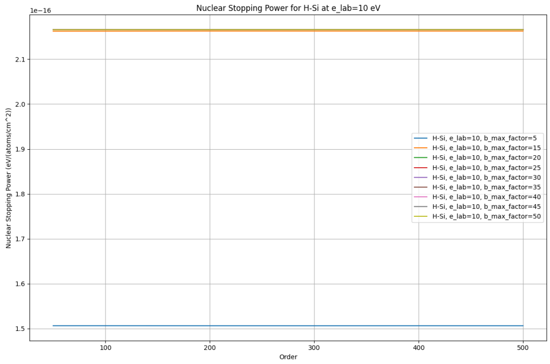
Note that the target for this test is to choose the minimal yet stable values of $b_{max} * a_u$ and order. If we look at figures b and c from 2, we will see $b_{max} * a_u$ converges at 15 and the order for Gauss–Legendre quadrature is saturated at 400. Similarly, for the $Si \rightarrow Au$ case, from figures f and g 2 we can say that at order = 200 and $b_{max} * a_u = 30$ converges.

Please note that for a successful integration, we need to set a good range of b. Even though the range should be from 0 to b_{max} to avoid the zero value error, we take the b_{min} value close to zero (1e-3).

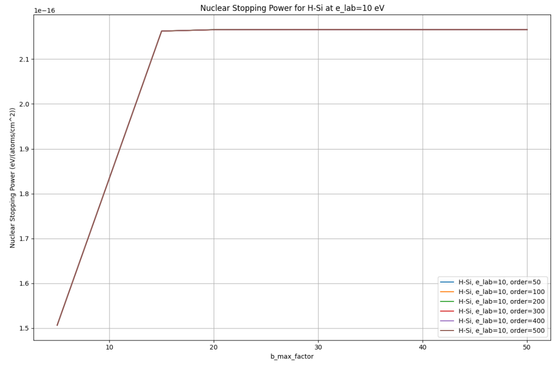
6.2 Difference between ZBL and Universal nuclear stopping power

Putting the value b_{max} and the order value from the convergence test, the simulation is run. The plotted figure in log-log space is shown in Figure 4. Even though the relative absolute difference varies in the energy range, we can see that the maximum relative difference is only **5.77 percent for $H \rightarrow Si$ collision and 4.48 percent for $Si \rightarrow Au$.** Note that the higher energy values give the maximum difference.

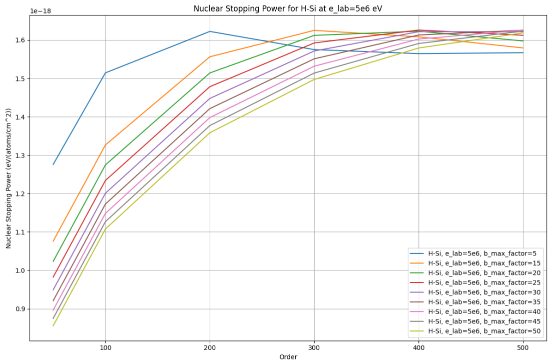
Also, we should keep in mind that the universal solution comes from an empirical fit from experimental data, and that can also be a cause of deviation. However, as this problem does not have an exact solution, we can't say this for sure.



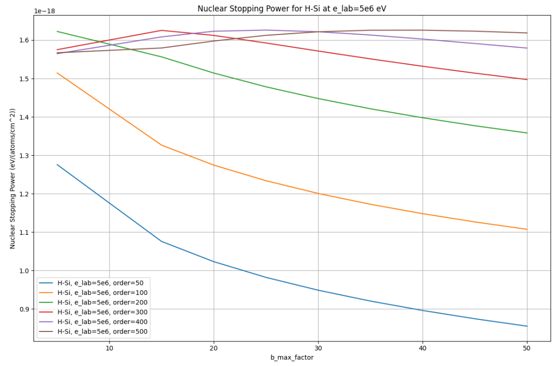
(a) S_n vs Order graph at 10 ev for H→ Si.



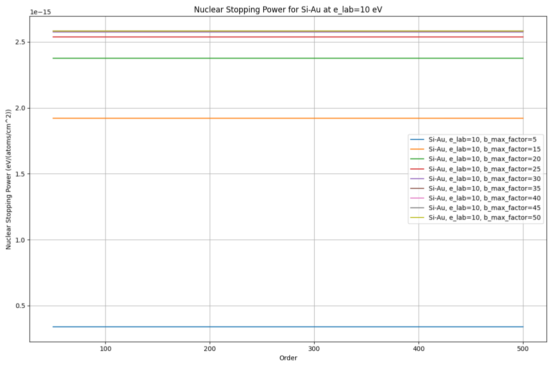
(b) S_n vs b_{max} graph at 10 ev for H→ Si.



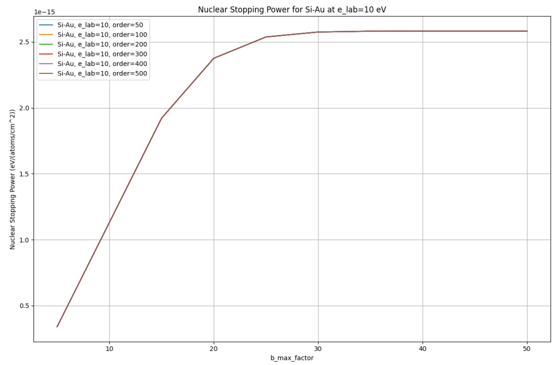
(c) S_n vs Order graph at 5e6 ev for H→ Si.



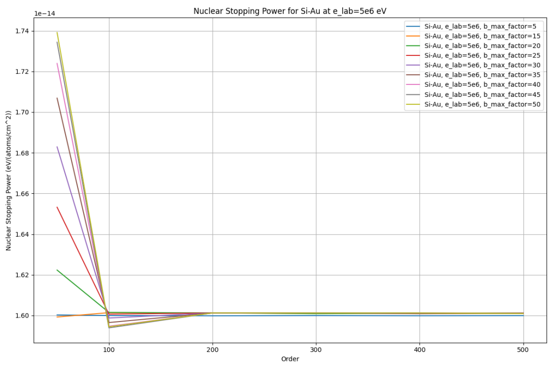
(d) S_n vs b_{max} graph at 5e6 ev for H→ Si.



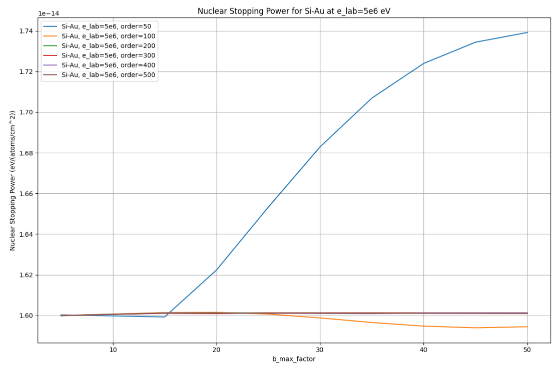
(e) S_n vs order graph at 10 ev for Si→ Au.



(f) S_n vs b_{max} graph at 10 ev for Si→ Au.



(g) S_n vs order graph at 5e6 ev for Si→ Au.



(h) S_n vs b_{max} graph at 5e6 ev for Si→ Au.

Figure 2: Convergence graphs of order and b$_{m}axat10evand5MevforH\rightarrow$Si and Si→Au nuclear power.

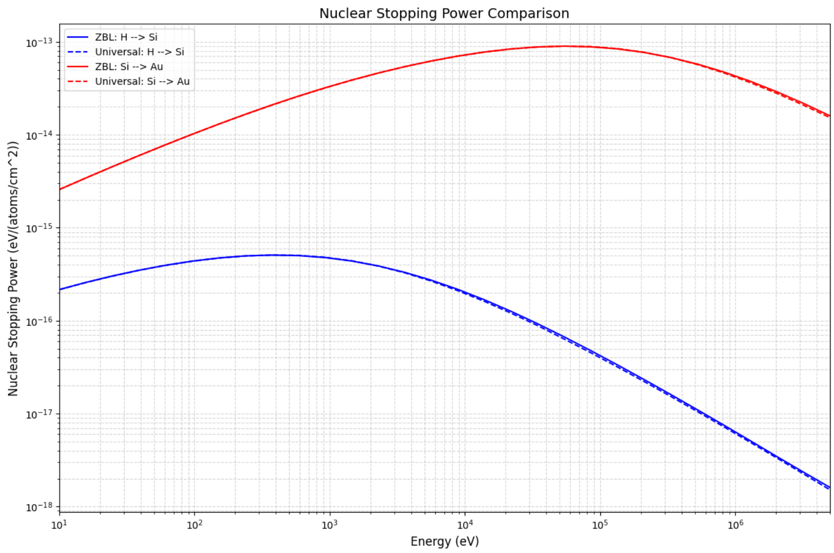


Figure 3: Relative difference in nuclear Stopping power of $H \rightarrow Si$ and $Si \rightarrow Au$

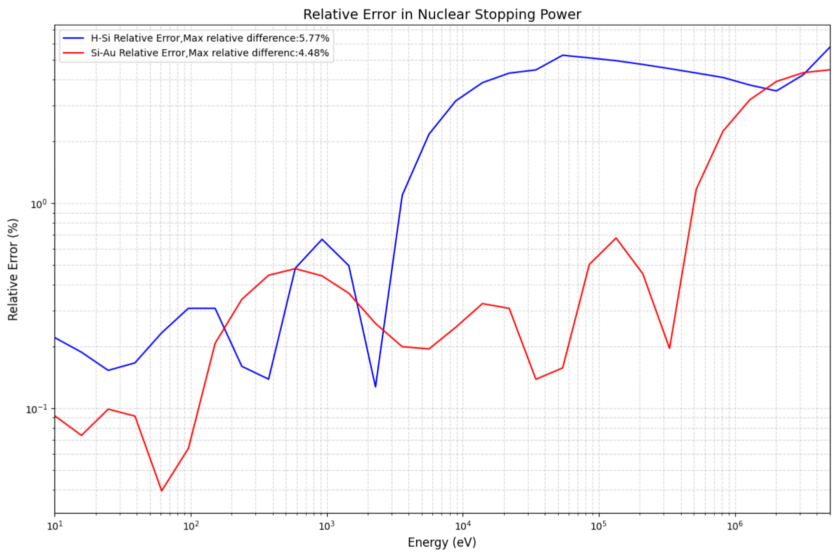


Figure 4: Relative difference in nuclear Stopping power of $H \rightarrow Si$ and $Si \rightarrow Au$

Even though this ZBL numerical solution works well for $H \rightarrow Si$ and $Si \rightarrow Au$ cases it takes a good amount of time for the calculation.

7 Conclusions

This comparative study of nuclear stopping power calculations demonstrates that the ZBL and universal models show excellent agreement (6 percent maximum relative difference). However, this is computationally expensive. Future work should focus on optimizing the computational efficiency by using better algorithms and programming languages, such as C++. Even though the ZBL model calculates at a greater computational cost, it gives good results. This makes it a good option when experimental results are not available. These findings provide clear guidance for selecting appropriate parameters and integration for stopping power models.

References

[1] Antti Kuronen and Aleksi Leino. *Lecture Notes on Numerical Methods of Scientific Computing.* Lecture notes. MATR322 Numerical Methods of Scientific Computing 2025, University of Helsinki. 2025.

[2] Wikipedia contributors. *Stopping power (particle radiation).* Accessed: 2025-05-17. 2024. URL: `https://en.wikipedia.org/wiki/Stopping_power_(particle_radiation)`.