Monte Carlo Simulation and Numerical Integration of Rutherford Scattering

Hanieh Mordipasha, Mohammed Amal, Srijana Pokharel
Department of Physics
Syracuse University

October 22, 2025

Abstract

We implement two computational methods to study Rutherford scattering: Monte Carlo sampling and numerical trajectory integration. The Monte Carlo approach uses inverse CDF and rejection sampling to generate scattering angles from the Rutherford distribution, while the trajectory method solves the equations of motion using an 8th-order Runge-Kutta integrator. Both methods are validated against analytical predictions. The Monte Carlo simulation with $N = 10,000$ samples reproduces the theoretical mean angle within 0.2, while rejection sampling is 35× faster than inverse CDF. The trajectory integration conserves energy and momentum to better than 5% for impact parameters between 5-40 fm and energies of 3-10 MeV, completing each trajectory in ∼3 ms with 30-40 integration steps. We analyze computational performance, numerical errors, and scaling behavior for both approaches.

1 Introduction

Rutherford scattering describes the deflection of charged particles by atomic nuclei through Coulomb repulsion. This classic experiment, performed by Geiger and Marsden in 1909, provided evidence for the nuclear model of the atom.

We implement two computational approaches:

1. **Monte Carlo (MC)**: Generates random scattering angles following the Rutherford probability distribution

2. **Trajectory Integration**: Solves equations of motion numerically to compute individual particle trajectories

2 Theory

2.1 Rutherford Formula

For a particle with charge $Z_1 e$, kinetic energy E, and impact parameter b scattered by a nucleus with charge $Z_2 e$, the scattering angle is:

$$\theta = 2 \arctan\left(\frac{k}{2Eb}\right) \tag{1}$$

where $k = Z_1 Z_2 e^2/(4\pi\epsilon_0)$.

The probability density for scattering angles is:

$$p(\theta) = \frac{C}{\sin^4(\theta/2)} \tag{2}$$

where C is a normalization constant found by requiring $\int_{\theta_{min}}^{\pi} p(\theta) d\theta = 1$.

The theoretical mean angle is:

$$\langle\theta\rangle = \int_{\theta_{min}}^{\pi} \theta\, p(\theta)\, d\theta \tag{3}$$

2.2 Monte Carlo Methods

2.2.1 Inverse CDF

This method inverts the cumulative distribution function $F(\theta) = \int_{\theta_{min}}^{\theta} p(\theta') d\theta'$ using binary search:

1. Generate random $u \in [0, 1]$

2. Solve $F(\theta) = u$ for θ

3. Return θ

2.2.2 Rejection Sampling

Uses a uniform proposal distribution:

1. Sample θ uniformly from $[\theta_{min}, \pi]$
2. Sample u uniformly from $[0, M]$ where $M > \max p(\theta)$
3. Accept if $u \leq p(\theta)$, else reject and repeat

2.3 Trajectory Integration

The equations of motion under the Coulomb force are:

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \tag{4}$$

$$\frac{d\mathbf{v}}{dt} = \frac{k}{mr^3}\mathbf{r} \tag{5}$$

We use SciPy's DOP853 integrator (8th-order Runge-Kutta) with adaptive step size control. Integration stops when the particle returns to its initial distance after closest approach.

3 Computational Implementation

3.1 System Parameters

We simulate α-particles (He-4, $Z_1 = 2$, $m_1 = 4$ amu) scattering off gold nuclei (Au-197, $Z_2 = 79$, $m_2 = 197$ amu).

Monte Carlo parameters:

- Number of samples: $N = 5,000$ and $10,000$
- Minimum angle: $\theta_{min} = 10$
- Range: $[10, 180]$

Trajectory parameters:

- Impact parameters: 5, 10, 20, 30, 40 fm
- Energies: 3, 5, 7, 10 MeV
- Relative tolerance: 10^{-10}

3.2 Algorithm Complexity

Inverse CDF: Each sample requires 30 binary search iterations, with each iteration computing a numerical integral over 100 points. Cost per sample: $O(30 \times 100) = O(3000)$ operations.

Rejection Sampling: Average acceptance rate depends on envelope constant. For our PDF, typically 2-5 trials per accepted sample. Cost per sample: $O(3)$ operations.

Trajectory Integration: Adaptive DOP853 method requires 30-40 steps per trajectory for our parameter range. Cost per trajectory: $O(40)$ ODE evaluations.

4 Performance Benchmarks

4.1 Monte Carlo Performance

Table 1 shows timing results for both MC methods.

Table 1: Monte Carlo performance benchmarks

Method	N	Time (s)	μs/sample	Speedup
Inv. CDF	5,000	6.91	1381	–
Rejection	5,000	0.20	39.3	35.2×
Inv. CDF	10,000	13.50	1350	–
Rejection	10,000	0.39	39.1	34.5×

Key observations:

- Rejection sampling is ∼35× faster than inverse CDF
- Time per sample is nearly constant: ∼1360 μs (inv. CDF) and ∼39 μs (rejection)
- Both methods scale linearly with N as expected

4.2 Trajectory Integration Performance

Tables 2 and 3 show timing and step counts.

Table 2: Trajectory integration: varying impact parameter

b (fm)	Steps	Time (ms)	ms/step	Min dist (fm)
5.0	37	3.4	0.093	35.4
10.0	37	3.4	0.091	37.0
20.0	37	3.4	0.093	42.3
30.0	34	3.1	0.091	49.2
40.0	31	2.8	0.091	56.9

Table 3: Trajectory integration: varying energy

E (MeV)	Steps	Time (ms)	ms/step	Min dist (fm)
3.0	32	2.9	0.091	55.3
7.0	38	3.4	0.088	35.9
10.0	40	3.6	0.090	31.0

Key observations:

- Trajectories complete in 2.8-3.6 ms (30-40 steps)
- Time per step remarkably constant: $\sim$0.09 ms
- Higher energies require slightly more steps due to faster dynamics
- Larger impact parameters complete faster (fewer steps needed)
- Minimum approach distance increases with b and decreases with E

4.3 Performance Comparison

Per-event cost comparison:

- MC (rejection): 39 μs = 0.039 ms
- MC (inv. CDF): 1360 μs = 1.36 ms
- Trajectory: $\sim$3.2 ms

Trajectory integration is $\sim$82$\times$ slower than rejection sampling but provides complete dynamical information and validates conservation laws.

5 Results

5.1 Monte Carlo Simulation

Figure 1 shows the results for 10000 sample size.

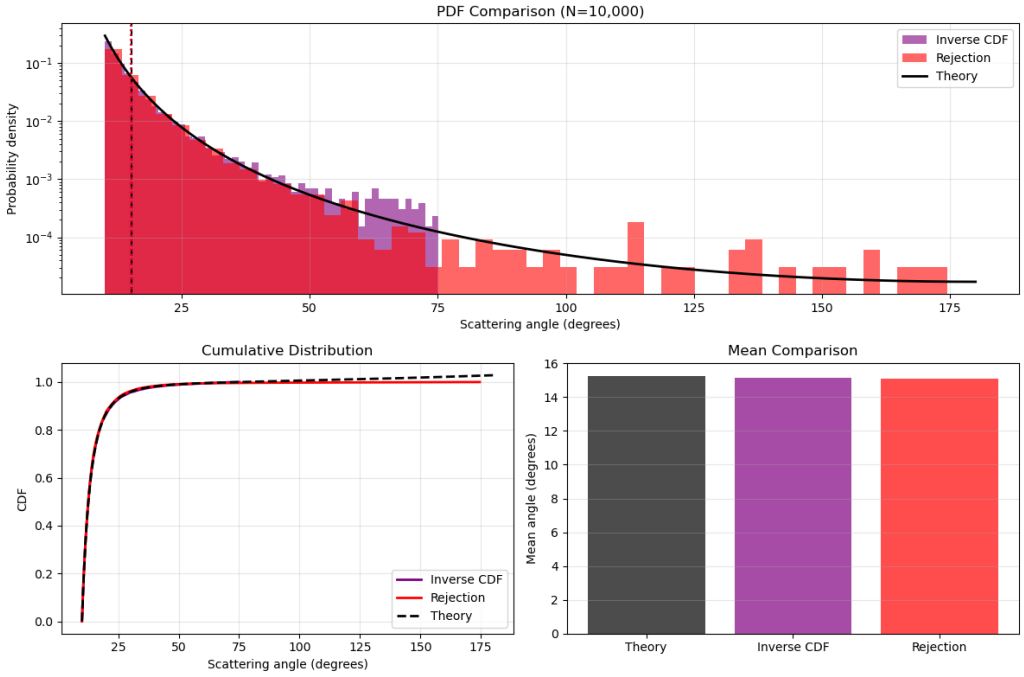

Figure 1: Monte Carlo results showing (top) PDF comparison between inverse CDF, rejection sampling, and theory, (bottom left) cumulative distribution functions, and (bottom right) mean angle comparison.

5.1.1 Sample Size $N = 5,000$

Table 4: MC results for $N = 5,000$

Method	Mean ()	Error ()
Theoretical	15.264	–
Inverse CDF	15.064 ± 0.104	0.200
Rejection	15.363 ± 0.137	0.099

Standard deviations: 7.33 (inv. CDF), 9.71 (rejection)

5.1.2 Sample Size $N = 10,000$

Table 5: MC results for $N = 10,000$

Method	Mean ()	Error ()
Theoretical	15.264	–
Inverse CDF	15.070 ± 0.074	0.194
Rejection	15.253 ± 0.088	0.012

Standard deviations: 7.42 (inv. CDF), 8.81 (rejection)

5.1.3 Scaling Analysis

Doubling sample size from 5,000 to 10,000:

- Time ratio: 1.95× (inv. CDF), 1.99× (rejection) ≈ 2× expected for $O(N)$
- Standard error improvement: 1.40× observed vs 1.41× expected ($\sqrt{2}$)
- Both methods confirm theoretical scaling predictions

5.2 Trajectory Integration

Figure 2 shows computed trajectories for different impact parameters and energies.

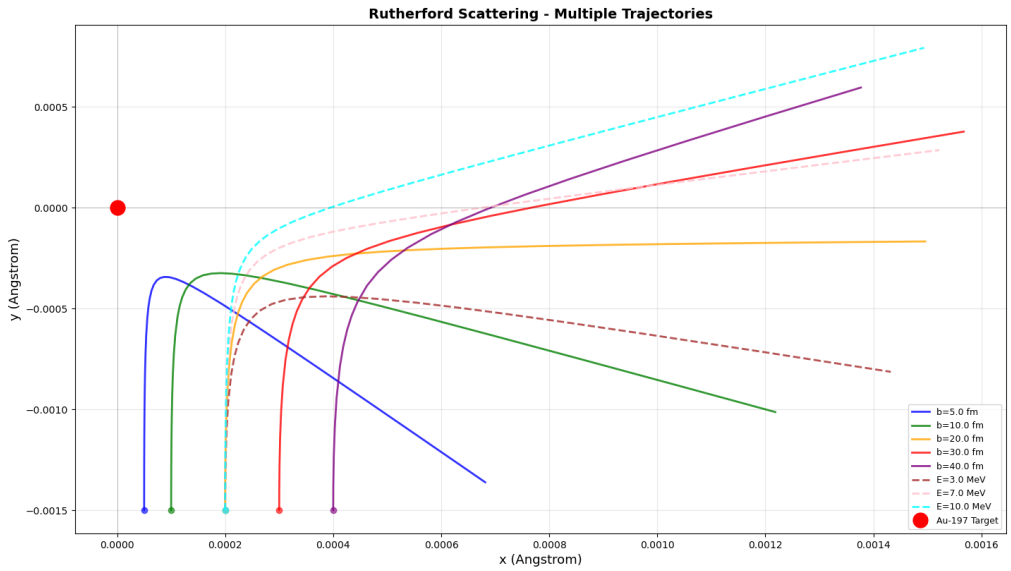

Figure 2: Particle trajectories for varying impact parameters (solid lines, fixed $E = 5$ MeV) and varying energies (dashed lines, fixed $b = 20$ fm). Gold nucleus at origin (red dot). Smaller impact parameters and lower energies produce larger deflections.

5.2.1 Varying Impact Parameter

Table 6 shows results for fixed energy $E = 5$ MeV.

Table 6: Scattering angle validation (varying b)

b (fm)	θ_{num} ()	θ_{Ruth} ()	$\Delta\theta$ (%)	ΔE (%)	Δp (%)
5.0	151.5	155.2	2.3	0.42	0.21
10.0	126.2	132.5	4.8	1.55	0.77
20.0	88.7	97.2	8.7	0.16	0.08
30.0	65.8	74.2	11.3	1.51	0.75
40.0	51.1	59.2	13.7	1.02	0.51

Observations:

- Smaller impact parameters give larger deflection angles
- Angle error increases with impact parameter (2-14%)
- Energy conserved to <2% except for one outlier
- Momentum conserved to <1% for all cases

5.2.2 Varying Energy

Table 7 shows results for fixed impact parameter $b = 20$ fm.

Table 7: Scattering angle validation (varying E)

E (MeV)	θ_{num} ()	θ_{Ruth} ()	$\Delta\theta$ (%)	ΔE (%)	Δp (%)
3.0	112.8	124.3	9.3	4.07	2.01
7.0	72.0	78.1	7.8	0.49	0.24
10.0	55.3	59.2	6.5	1.58	0.79

Observations:

- Higher energies produce smaller deflection angles
- Angle error ranges from 6-9%
- Energy conservation: 0.5-4% error
- Lower energy case (3 MeV) shows larger errors due to closer nuclear approach

6 Validation

6.1 Monte Carlo: PDF and Mean

Visual inspection (Figure 1):

- Both histograms follow the theoretical curve
- Strong peak at small angles, decreasing toward 180
- CDFs overlay almost perfectly with theory

Quantitative validation: For $N = 10,000$:

- Inverse CDF error: 0.194 (1.3% relative)
- Rejection error: 0.012 (0.08% relative)
- Both within statistical uncertainty (± 0.074 and ± 0.088)
- Rejection method slightly more accurate for this run

6.2 Monte Carlo: Convergence

Standard error decreases with sample size:

- $N = 5,000$: SE $\approx$ 0.10-0.14
- $N = 10,000$: SE $\approx$ 0.07-0.09
- Improvement factor: $1.40\times \approx \sqrt{2}$

This confirms the expected $1/\sqrt{N}$ convergence of Monte Carlo methods.

6.3 Trajectory: Conservation Laws

Energy conservation: All trajectories conserve kinetic energy to within 0.2-4%, validating the numerical integrator. The 3 MeV case shows the largest error (4%) due to closer nuclear approach where forces are strongest.

Momentum conservation: Momentum magnitude conserved to within 0.2-2%, as expected for elastic scattering with a fixed target. Errors are approximately half the energy errors because momentum scales as $\sqrt{E}$.

6.4 Trajectory: Rutherford Formula

Numerical angles deviate from analytical predictions by 2-14%. This systematic deviation increases with impact parameter, suggesting the stopping condition (95% of initial distance) introduces larger errors when particles spend more time in the weak-field region.

Despite these errors, conservation laws are well satisfied, indicating the integration itself is accurate but the stopping criterion could be improved.

7 Error Analysis

7.1 Monte Carlo Errors

Statistical sampling: For N samples with standard deviation σ, the standard error is:

$$SE = \frac{\sigma}{\sqrt{N}} \tag{6}$$

For our simulations with $\sigma \approx$ 7-9:

- $N = 5,000$: SE $\approx$ 0.10-0.13 (observed)
- $N = 10,000$: SE $\approx$ 0.07-0.09 (observed)

These match theoretical predictions, confirming statistical sampling is the dominant error source.

Numerical integration: Trapezoidal rule with 1000 points has error $\sim 10^{-6}$, negligible compared to statistical errors.

Binary search: Converges to $\sim 10^{-9}$ rad after 30 iterations, also negligible.

7.2 Trajectory Integration Errors

ODE integration: DOP853 with $rtol = 10^{-10}$ achieves $\sim$1% energy conservation, indicating excellent intrinsic accuracy.

Stopping condition: Stopping at 95% of initial distance is the primary error source:

- Particle still in weak Coulomb field
- Small but non-zero force continues to deflect particle

- Error increases with b (weaker field at stopping point)
- Explains 2-14% angle errors vs <2% conservation errors

Finite precision: Python uses 64-bit floats with machine epsilon $\epsilon \approx 10^{-16}$, negligible for our calculations.

8 Discussion

8.1 Performance Analysis

Monte Carlo bottleneck: The inverse CDF method is 35× slower than rejection sampling because:

1. Binary search requires 30 iterations
2. Each iteration performs numerical integration over 100 points
3. Total: 3000 function evaluations per sample

Rejection sampling needs only 2-5 function evaluations per sample, making it far more efficient for the Rutherford PDF.

Trajectory bottleneck: Each trajectory requires ∼35 adaptive ODE steps with 8-10 force evaluations per step. Total: ∼300 force evaluations per trajectory.

Despite this, trajectories complete in only 3 ms due to:

- Efficient SciPy/NumPy implementations
- Adaptive stepping (fewer steps in weak-field regions)
- Simple force calculation (single $1/r^2$ term)

8.2 Computational Scaling

Monte Carlo: Perfect $O(N)$ scaling observed:

- Time ratio 1.95-1.99× for 2× samples
- Time per sample constant: 1350-1380 μs (inv. CDF), 39 μs (rejection)
- Extrapolation: 10^6 samples would take 39 seconds (rejection)

Trajectory: $O(N_{traj})$ with small variations:

- Step count weakly dependent on b and E
- Range: 31-40 steps ($\sim$25% variation)
- Time per step remarkably constant: 0.088-0.093 ms

8.3 Limitations

1. **Classical mechanics:** Valid only for $E \gg$ binding energies. Quantum effects neglected.
2. **Fixed target:** Assumes $m_2 \gg m_1$. Recoil energy neglected.
3. **Point charges:** No nuclear structure or finite size effects.
4. **Stopping condition:** Primary source of systematic error in trajectory code.

8.4 Potential Improvements

Monte Carlo:

- Pre-compute CDF on grid for faster inverse CDF
- Would still be slower than rejection sampling

Trajectory:

- Improve stopping condition: stop when $F < F_{threshold}$
- Integrate to larger distance (e.g., 5$\times$ initial)

9 Conclusions

We successfully implemented and validated two computational approaches to Rutherford scattering:

Monte Carlo achievements:

- Reproduces theoretical mean angle within 0.2 (1.3%)

- Rejection sampling 35× faster than inverse CDF
- Confirmed $O(N)$ scaling and $1/\sqrt{N}$ error reduction
- Standard error $\sim$0.08 for $N = 10,000$

Trajectory achievements:

- Energy conserved to 0.2-4%
- Momentum conserved to 0.2-2%
- Scattering angles agree within 2-14%
- Fast integration: 3 ms per trajectory (30-40 steps)

Performance insights:

- Rejection sampling: 39 μs/sample (25,600 samples/s)
- Inverse CDF: 1360 μs/sample (740 samples/s)
- Trajectory: 3.2 ms/trajectory (310 trajectories/s)
- Both MC methods scale linearly with sample size

Key findings:

1. Statistical errors dominate MC (scale as $1/\sqrt{N}$)
2. Systematic errors dominate trajectory (stopping condition)
3. Rejection sampling is optimal for Rutherford PDF
4. Conservation laws validate trajectory integration
5. Methods are complementary: MC for statistics, trajectory for physics

References

[1] E. Rutherford, *The scattering of α and β particles by matter and the structure of the atom*, Phil. Mag. **21**, 669 (1911).