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Modeling ion-neutral collisions using 'universal' scattering for drifting plasmas or ion beams in PIC-DSMC codes.

ALEPH
Advanced Plasma Transport & Kinetics

PRESENTED BY

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Outline

Theory
- Elastic scattering and nuclear stopping power
- Universal scattering cross section
- Interactions in PIC-DSMC

Implementation
- Cross section calculation and sampling
- Integration vs tables

Example
- Ions through background gas

Validation of calculated cross sections
- High energy ~MeV
- Low energy ~10eV

Code-to-Code comparison
- Aleph vs SRIM

Conclusion and Questions

Kinetic Plasma Simulations in Aleph

Sandia owned- PIC-DSMC ES code for kinetic simulation of low temperature and non-equilibrium plasmas

Some features:

- Collisional Vlasov-Poisson Solver
- Massive parallelization for running on large supercomputers
- Unstructured mesh
- 2B element problems ran, 10-100B possible
- Extensive diagnostic outputs
- Advanced BC's, chemistry, …

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Test bed for PIC-DSMC ion-neutral scattering

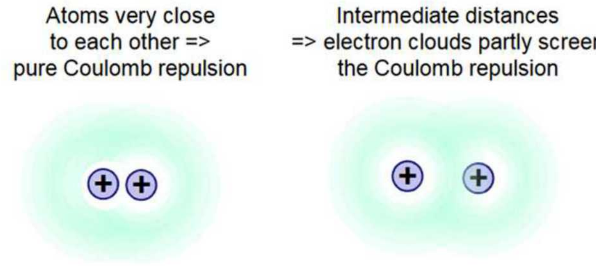
Purpose:

Modeling interactions in PIC-DSMC codes requires accurate cross sections

$$N_c = N_i \sigma_T \rho_g v_r \Delta t$$

Scattering cross section data is scarce

- Drifting plasmas and ion beams
- Intermediate energy of 10eV to 100keV



Lack of data is typically dealt with by extrapolation from low/high energy

Accurate elastic differential cross sections for

- Integral elastic (probability of collision)
- Momentum transfer
- Viscosity

$$\sigma_{el} = 2\pi \int_0^\pi d\theta \sin\theta \frac{d\sigma}{d\Omega}$$

$$\sigma_{vi} = 2\pi \int_0^\pi d\theta \sin^3\theta \frac{d\sigma}{d\Omega}$$

$$\sigma_{mt} = 2\pi \int_0^\pi d\theta \sin\theta (1 - \cos\theta) \frac{d\sigma}{d\Omega}$$

Accurate knowledge of energy transfer can elucidate elastic/inelastic interdependencies and avoid the potentially double counting interactions

Enable a physics based approach to calculate scattering cross section for modeling of ion-neutral collisions in plasmas

*Krstić, P. S., & Schultz, D. R. *Physical Review A*, *60*(3) 2118.

Elastic Scattering

Orbit Equation

$$\Theta = \pi - 2p\int_{r_0}^{\infty} [r^2 g(r)]^{-1} dr,$$

$$g(r) = \sqrt{1 - \frac{V(r)}{E_r} - \frac{p^2}{r^2}}.$$

Analytic solutions for:

Hard Sphere

$$V(r) = \begin{cases} 0 & r > R \\ \infty & r < R \end{cases}$$

Coulomb-like potentials

$$V(r) = \frac{Z_1 Z_2 e^2}{r^2}$$

$$V(r) = \frac{Z_1 Z_2 e^2}{r}$$

Rutherford scattering formula

$$\frac{d\sigma}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{16\pi\varepsilon_0 E_0}\right)^2 \frac{1}{\sin^4(\frac{\theta}{2})}$$

Great success!
- Light ion on heavy-target collisions
- Bare Coulomb interaction

Screened Coulomb potentials relevant for medium-to-low energy collisions

$$V(r) = \frac{Z_1 Z_2 e^2}{r}\Phi\left(\frac{r}{a}\right) \qquad \Phi\left(\frac{r}{a}\right) = \sum_i^n c_i exp^{(-d_i \frac{r}{a})}$$

Something like Rutherford differential scattering formula would be ideal
- Low to medium energy interactions (10eV to 100keV)
- Screened Coulomb potentials

Universal Scattering Cross Section

From LSS*:

$$d\sigma = \pi a^2 \frac{f(t^{1/2})}{2t^{2/3}} dt \qquad t^{1/2} = \varepsilon \sin(\frac{\Theta}{2}).$$

- Rutherford-like at high energies
- Screened at medium to low energies
- Screening functions fitted

$$f(t^{1/2}) = \Lambda t^{1/2-m} \left[1 + (2\lambda t^{1-m})^q\right]^{1/q}$$

- Relationship to stopping power

$$S_n(\varepsilon) = \frac{1}{\varepsilon} \int_0^{\varepsilon} f(t^{1/2}) d(t^{1/2})$$

Nr. 14 9

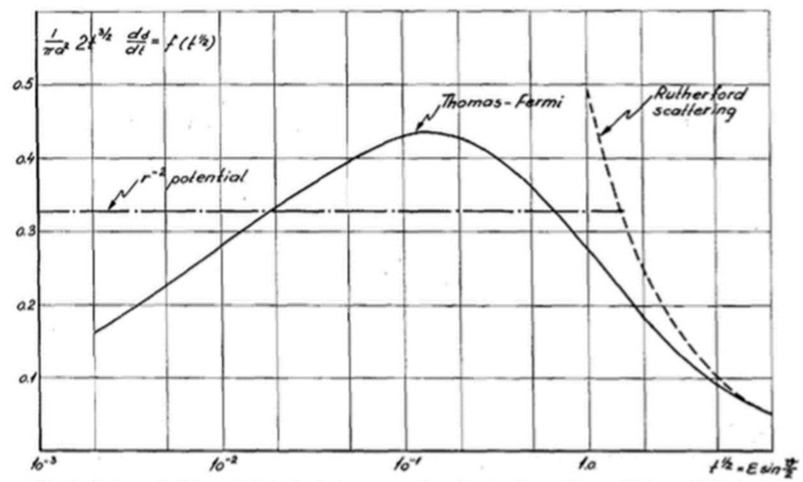
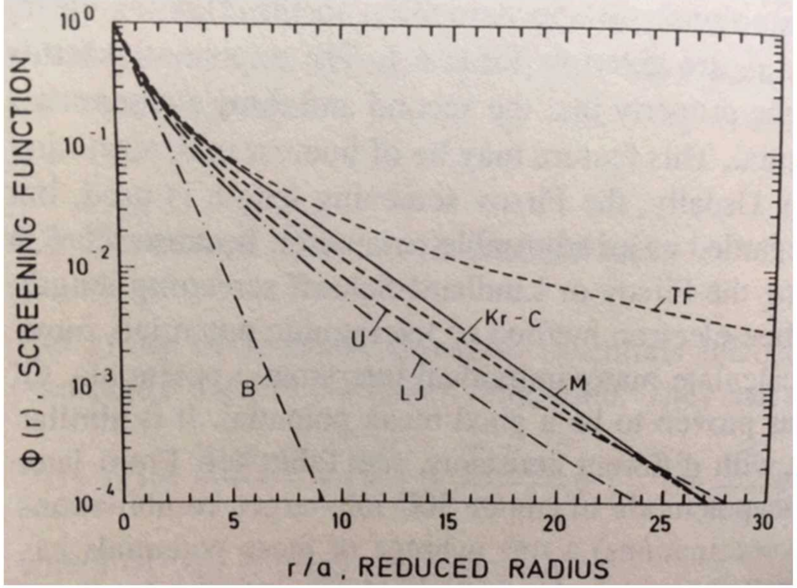


Fig. 1. Universal differential scattering cross section for elastic nuclear collisions, (2.9), based on a Thomas-Fermi type potential. At high values of $t^{1/2}$ it joins smoothly the Rutherford scattering. The cross section corresponding to power law scattering (2.6), or (2.6'), with $s = 2$ is also shown.



Which fit to use? … Which one is sufficiently accurate?

*Linhard, Nielsen, & Scharff (1963), Linhard, Scharff & Schiott (1962)

Use the ZBL potential

Nuclear stopping data scaling based on physical arguments

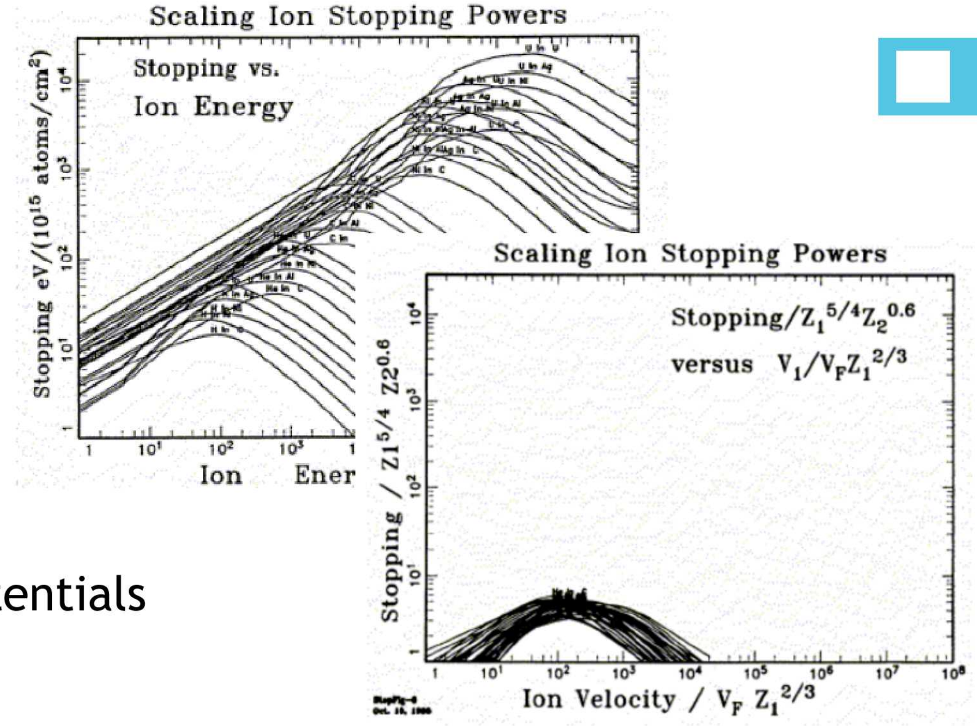
ZBL is the best fit to:

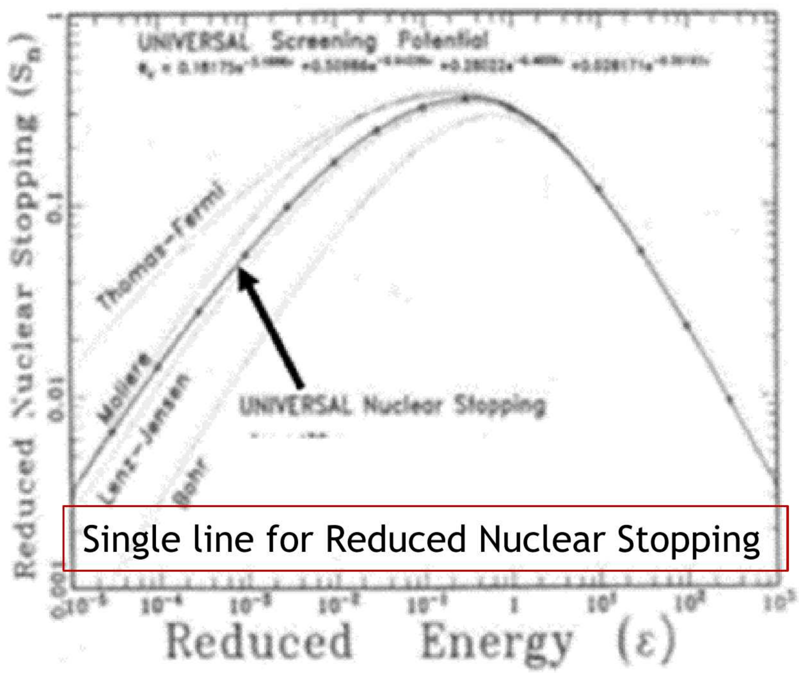
- HF calculations of interatomic potentials
- Reduced nuclear stopping data

Sometimes called ‘average’ potential

Validated: derived from experimental stopping data

ZBL potential is
- used in SRIM
- Accurate (within 10%)
- *Universal*





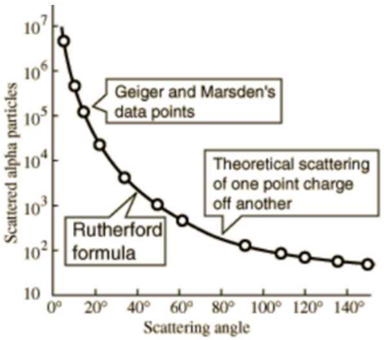
Quadrature → Avoid

Orbit equation computationally expensive, details unknown

$$\Theta = \pi - 2p \int_{r_0}^{\infty} [r^2 g(r)]^{-1} dr,$$

Differential scattering integral divergent

$$\sigma_{el} = 2\pi \int_0^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega};$$



ZBL suggested approaches

$$\cos\left(\frac{\Theta}{2}\right) = \frac{B + R_C + \Delta}{R_0 + R_C}$$

1. Magic Formula
2. Invert reduced nuclear stopping

$$f(x) = \frac{d}{dx}[xS_n(x)] \qquad d\sigma = \pi a^2 \frac{f(t^{1/2})}{2t^{2/3}} dt$$

Use analytical methods and reduced nuclear stopping function for elastic differential scattering cross section

Implementation: Scattering Tables

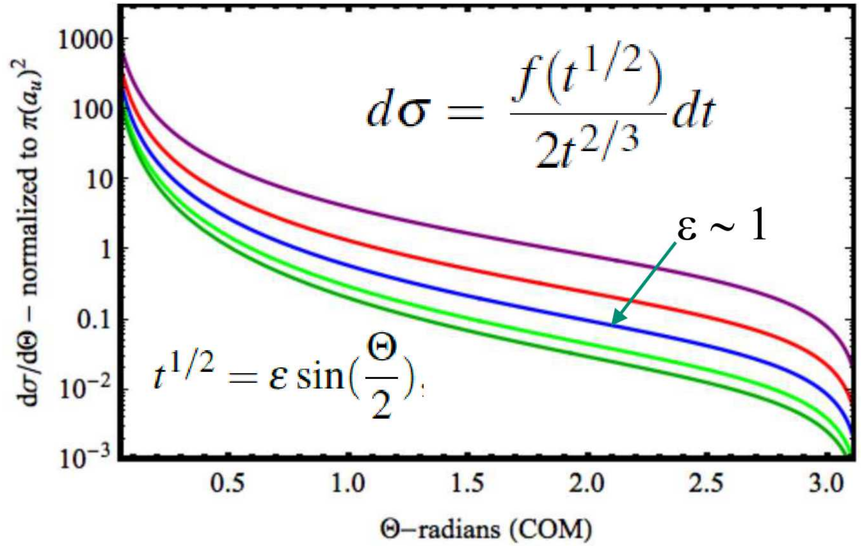
In terms of reduced quantities, calculation is agnostic of collision pair details

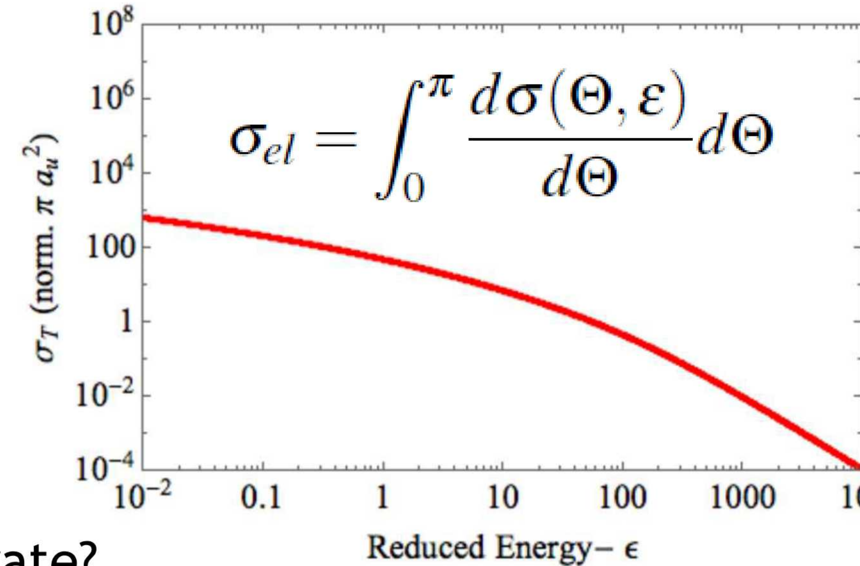
Enables the user to precompute tables before runtime!

Take advantage of fast table look up and interpolation
- 12 operations

In practice, the integral elastic cross section is truncated with a threshold angle of 0.01 radians in the COM frame

THAN-then-trapezoidal Rule





User-friendly, one free parameter, accurate?

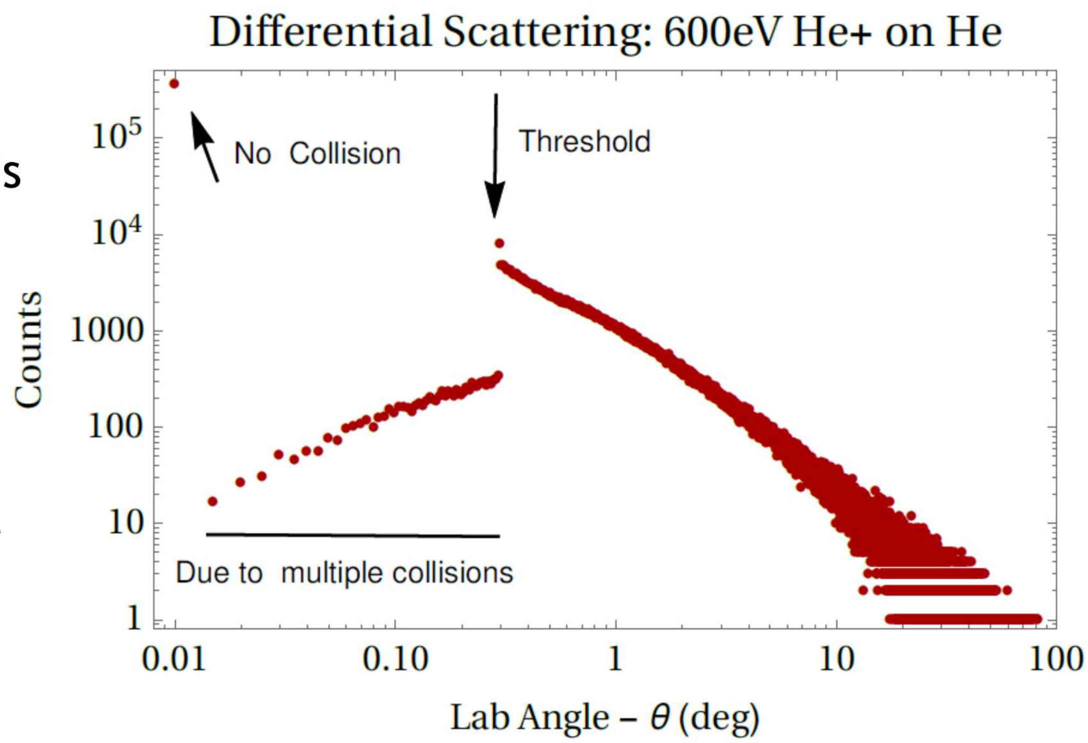
Results

- He^+ thru background He gas
- Sim is 1D3V
- 1M He^+ ions
- Fix density so that, domain is 1 mfp in length.

- Clear artifacts due to threshold

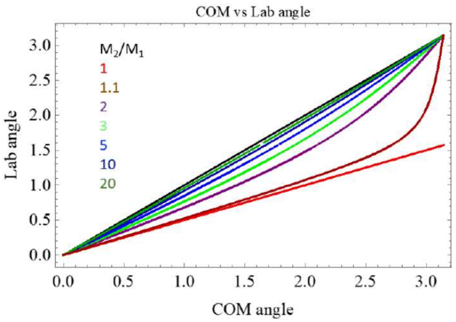
- Poisson statistics: expect 1M collisions

- Beer-Lambert: expect 63% beam attenuation



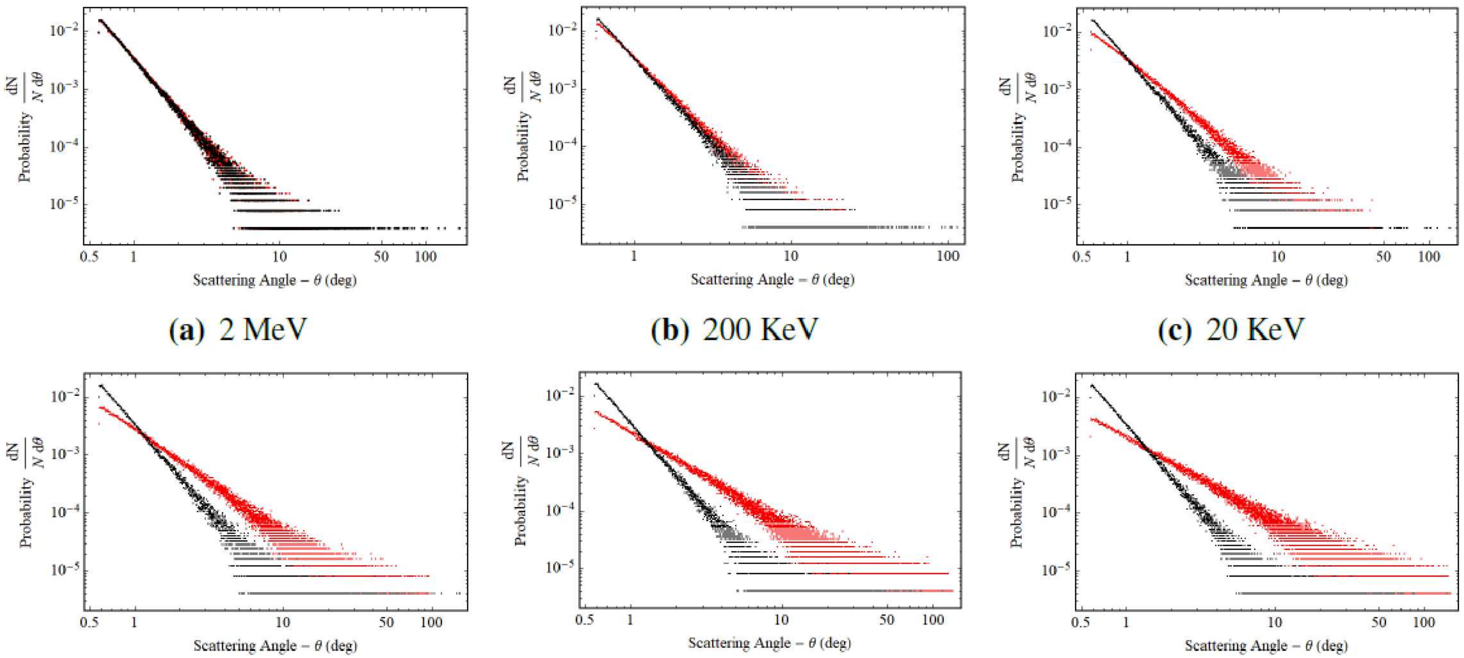
Algorithm captures the stochastic aspect of interactions and the expected beam attenuation

Compare to Rutherford



Choose a heavy target
- He on Ne

Differential Scattering



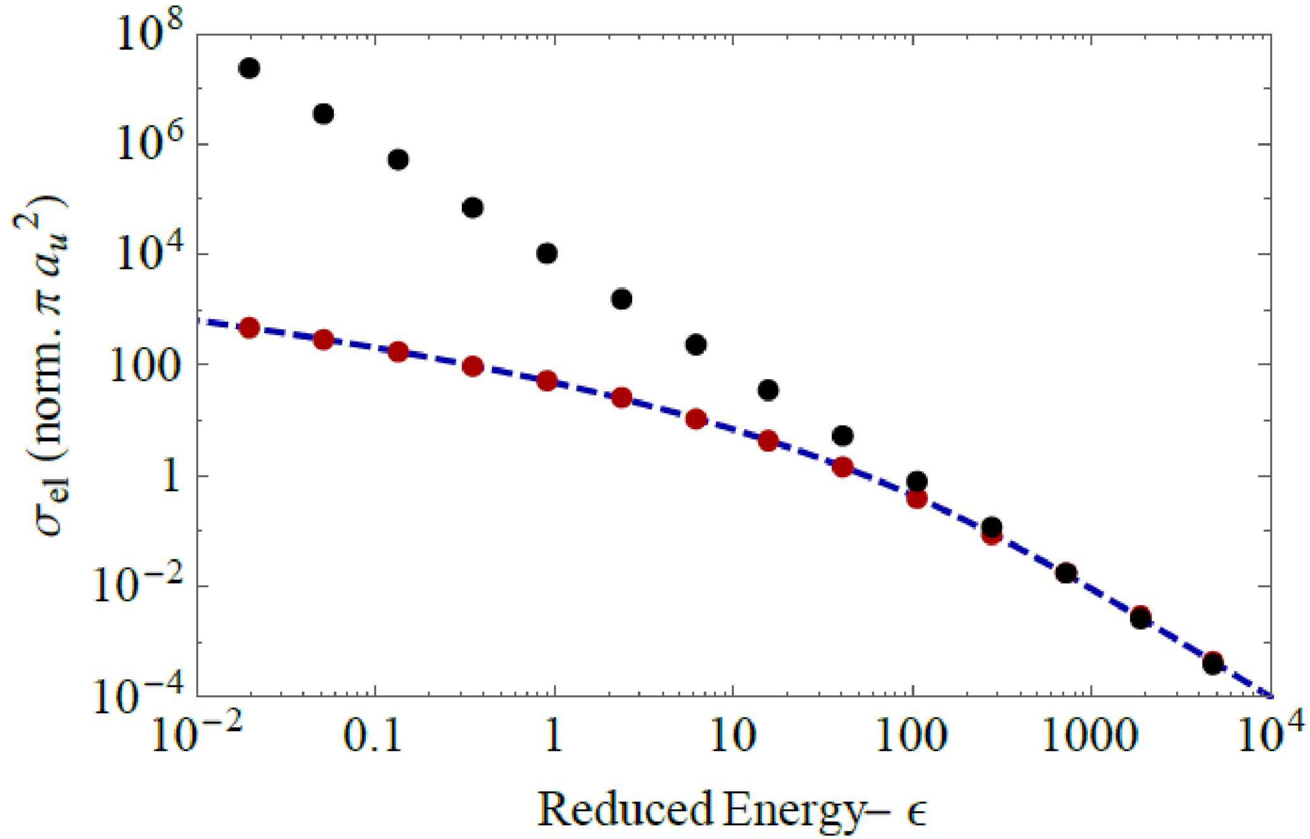
(a) 2 MeV (b) 200 KeV (c) 20 KeV

(d) 2 KeV (e) 200 eV (f) 20 eV

Good agreement for high energies

Compare to Rutherford

$$\sigma_{el} = \int_0^{\pi} \frac{d\sigma(\Theta,\varepsilon)}{d\Theta} d\Theta$$



Good agreement for high energies

Differential scattering at low energies: good data from the 60's

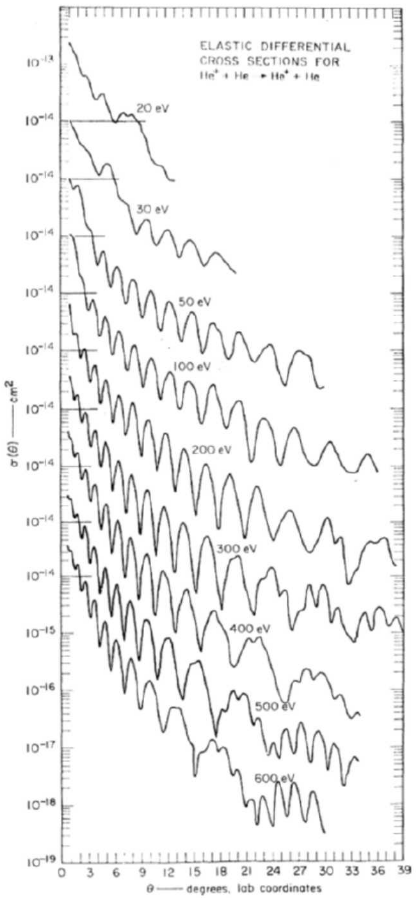


FIG. 6. Elastic differential scattering cross sections for He^+ on He at incident energies from 20 to 600 eV. Note the shifted scale; the proper scale is identified at 10^{-14} cm^2 by the intersection of a horizontal line with each curve.

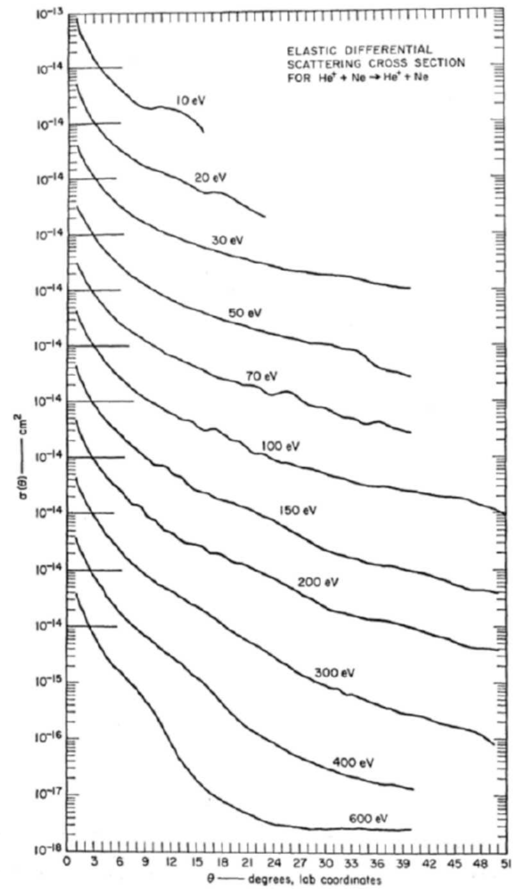
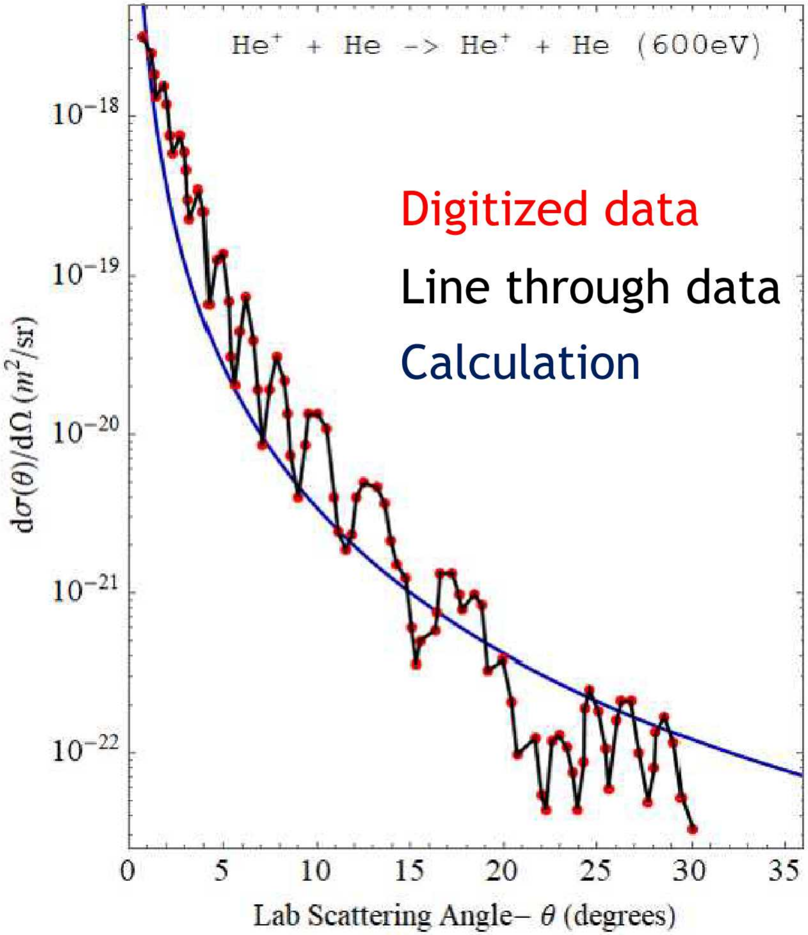
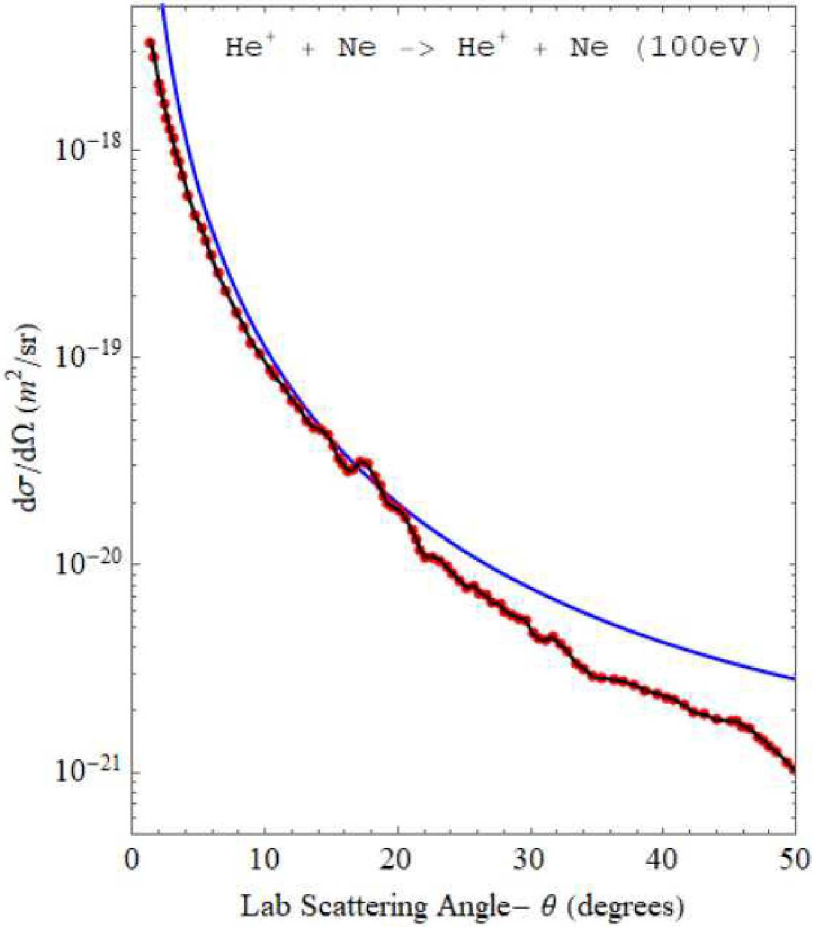


FIG. 8. Elastic differential scattering cross sections for He^+ on Ne at incident energies from 10 to 600 eV. Note the shifted scale; the proper scale is identified at 10^{-14} cm^2 by the intersection of a horizontal line with each curve.

W. Aberth and D. C. Lorents. Physical Review, 144(1):109, 1966.

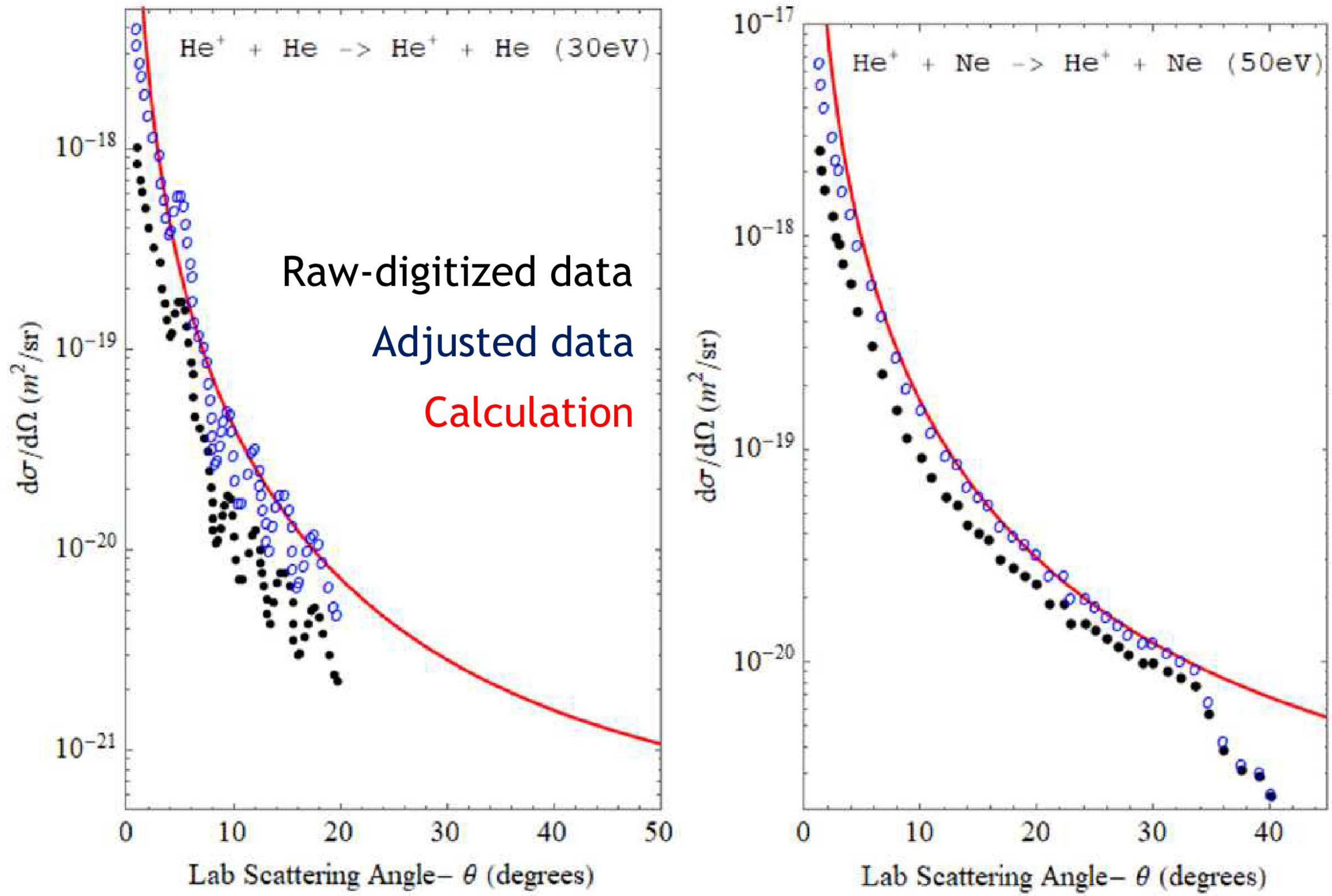
Compare to low energy scattering data





Good agreement at low energies

Compare to scattering data below 100eV



Agreement to within 5x or better

Integral Elastic Scattering Cross Section

Vahedi, Surrendra

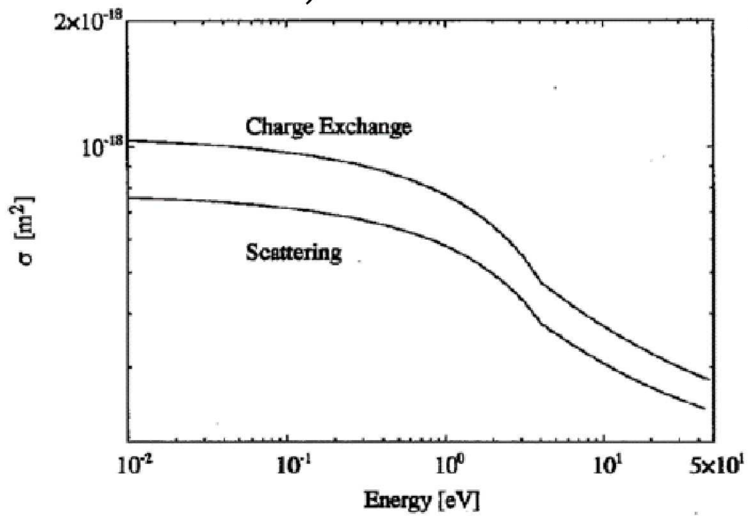
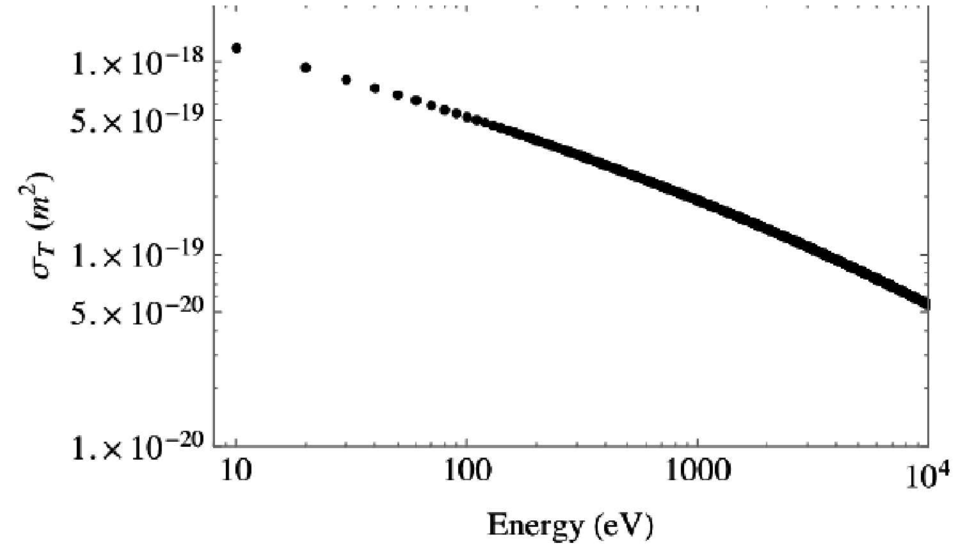


Fig. 5. The ion–neutral cross sections in argon.



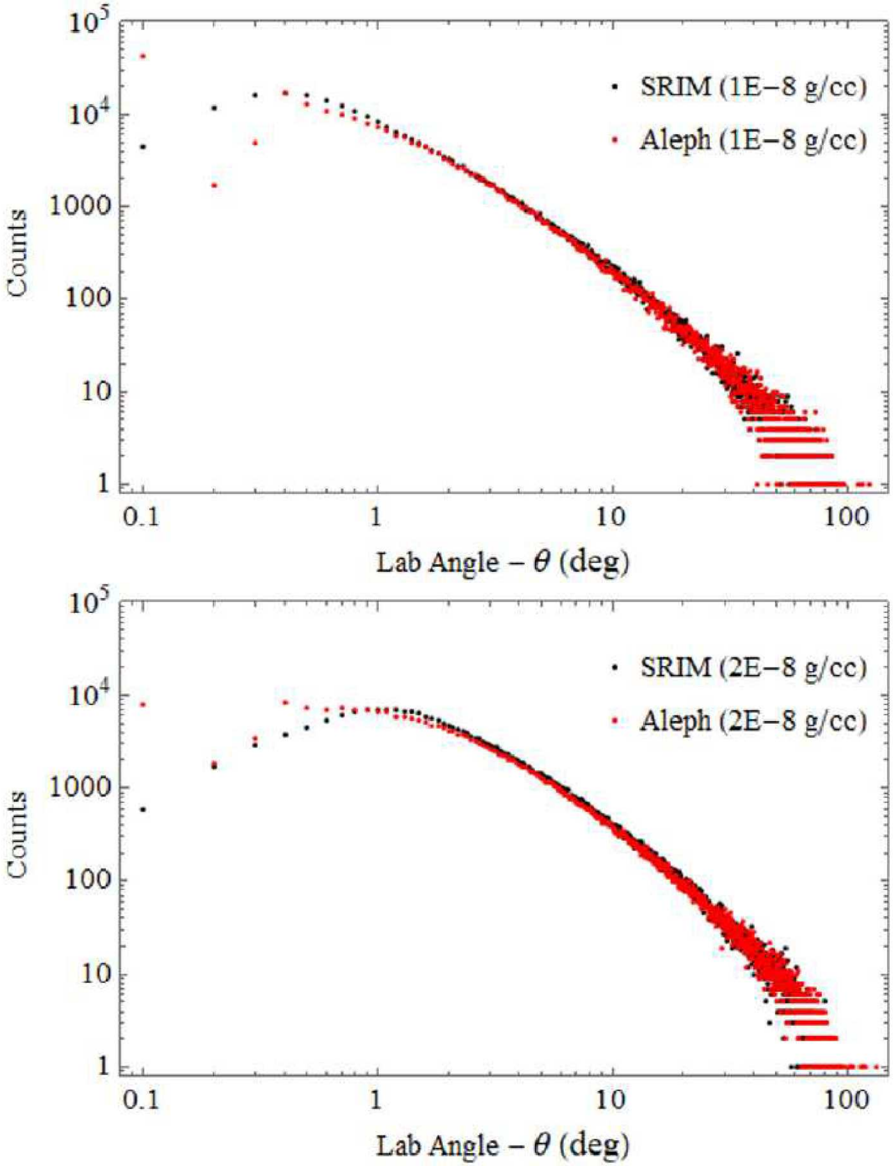
Direct comparison of values: 3x10^-19 vs 1.2x10^-18 m^2 for our calculation

However, choosing the same angular range of 6º and 174º, our calculation yields 3.45x10^-19

Important to calculate collisions for which are defined in the angular range of the integral cross section

Last but not least: Comparison to SRIM

- 600 eV He+ through He gas
- Scattering details are identical
- Implementation details show different artifacts



- A method to SRIM-like calculations in a PIC-DSMC setting
- Although not ideal for SRIM-like calculations, enables a similar capability in massively parallel platforms

Questions