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The Integration of Improved Monte Carlo Compton Scattering Algorithms Into The Integrated TIGER Series

Student Symposium Presentation

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Thomas J. Quirk IV
University of New Mexico
Student Intern

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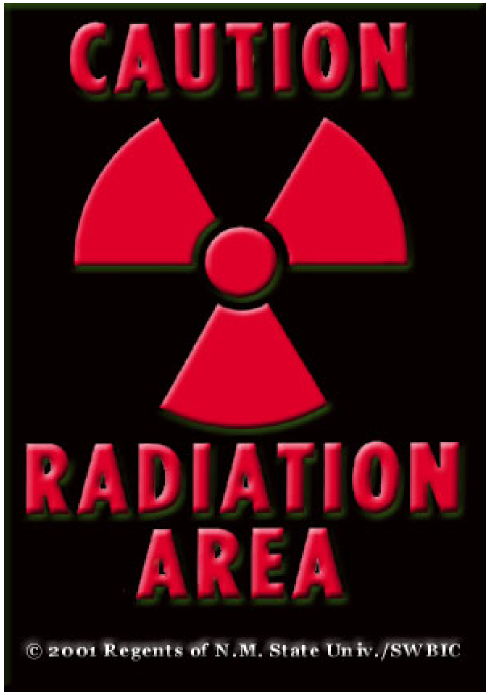
OVERVIEW

- Integrated TIGER Series (ITS)
- Introduction to Monte Carlo Methods
- Radiation Physics
  - Interactions
  - Compton Scattering
  - Doppler Broadening
- Compton Scattering Algorithm
- Results
- Future Work
- Conclusions



INTEGRATED TIGER SERIES (ITS)

- **ITS is a 3-D Monte Carlo code that simulates coupled electron/photon transport in continuous energy space from 1 keV to 1 GeV.**
- **Photon transport is modeled using analog tracking.**
- **Electron transport is modeled using Condensed History Methods.**

INTRODUCTION TO MONTE CARLO

“The essence of the method is to create games of chance whose behavior and outcome can be used to study an interesting (and often times complicated) phenomena.”

-Malvin H. Kalos, Monte Carlo Methods

RADIATION PHYSICS - INTERACTIONS

- **Photo-electric Effect**
  - Predominately low energy, high-Z phenomenon
  - Atom “absorbs” photon and emits electrons
- **Compton Scattering**
  - Intermediate energy range (0.1 to ~5 MeV)
  - Photon incoherently scatters off of atomic electron
- **Pair Production**
  - Electron and positron pair produced from highly energetic photon
  - Threshold energy of 1.022 MeV*, high-Z preference
  - Must occur in the presence of the nucleus to conserve momentum of incoming photon

RADIATION INTERACTION

CROSS SECTIONS

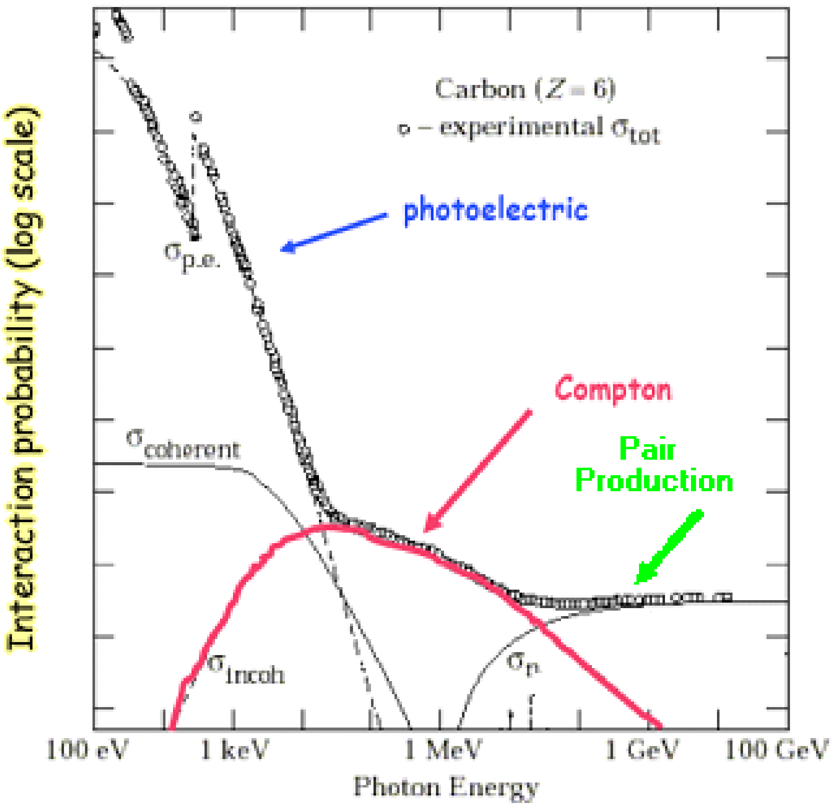
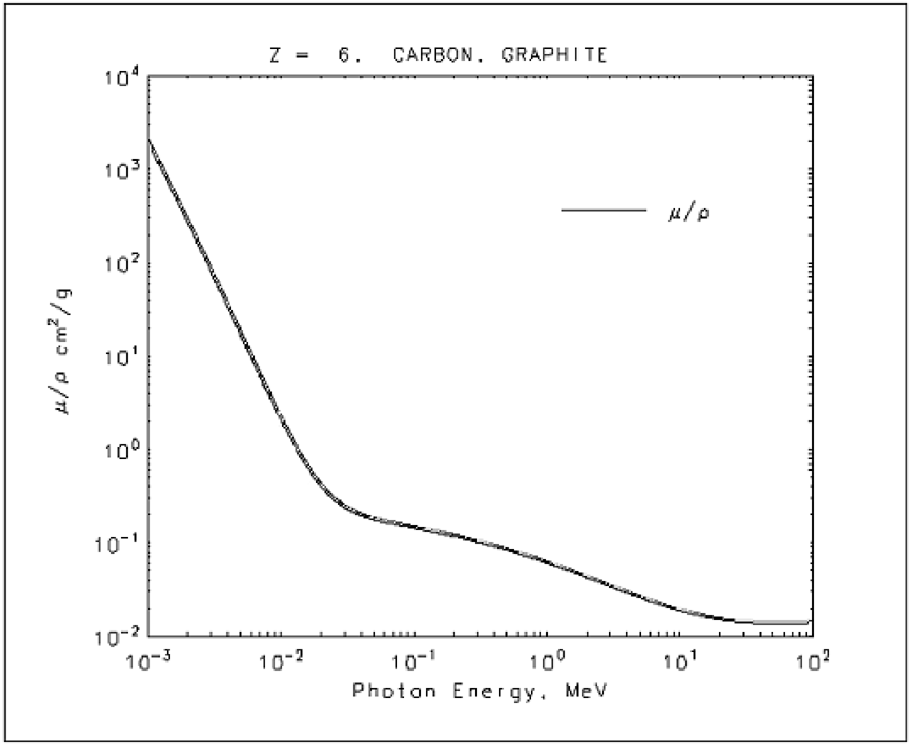


IMAGE SOURCE: http://www.physics.umanitoba.ca/~gwinner



http://physics.nist.gov/PhysRefData/XrayMassCoef/

COMPTON SCATTERING

In “academic” Compton scattering a photon strikes a free electron, initially at rest, and recoils with a lengthened wavelength identically prescribed by two-body Klein-Nishina kinematics.

$$\frac{d\sigma}{d\Omega} = Z\,\frac{r_e^2}{2}\left(\frac{E_C}{E}\right)^2 X_{KN}$$

$$X_{KN} = \left(\frac{E_c}{E} + \frac{E}{E_c} - \sin^2\theta\right)$$

$$E_{Compton} = \frac{E}{1 + \frac{E}{mc^2}(1-\cos\theta)}$$

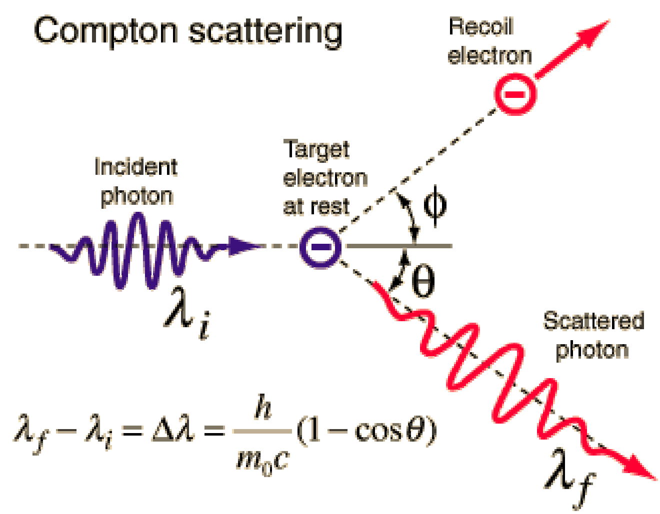


IMAGE SOURE: http://hyperphysics.phy-astr.gsu.edu

COMPTON SCATTERING

"Real" Compton scattering is complicated by:

- Binding effects
  - Electron or atom recoil?
  - Electron/orbital selection is important
- Doppler broadening
  - Electron has initial momentum
- Quantum mechanics
  - Statistical uncertainty implicit to atomic systems

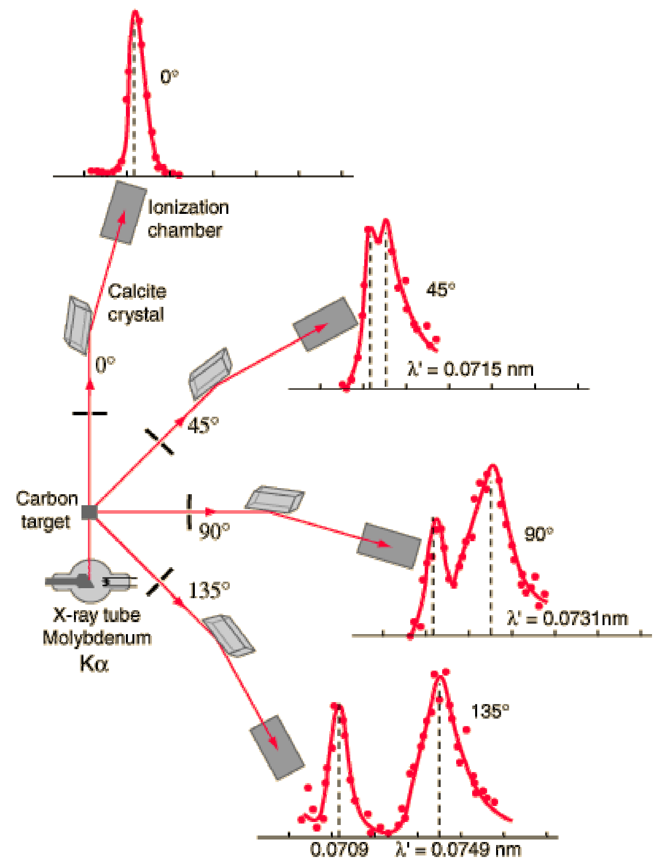


IMAGE SOURE: http://hyperphysics.phy-astr.gsu.edu

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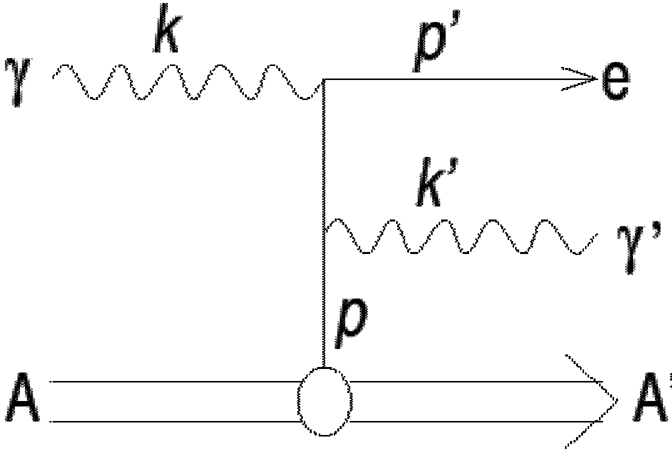
MODELING COMPTON SCATTERING

Reality is relaxed by the Impulse Approximation (IA) under the following assumptions:

- Instantaneous momentum transfer to electron
- Unpolarized photons
- Photon energy is greater than binding energy
- Electron’s potential is spatially independent (within orbital)
- Electrons are scatter in plane waves such that: $E = \hbar c k$



MODELING COMPTON SCATTERING

Klein-Nishina distribution is modified by IA:

(total cross sections remain unchanged)

$$\frac{d\sigma}{dE' d\Omega} = \frac{r_e^2}{2}\left(1+\left(\frac{p_z}{mc}\right)^2\right)^{-\frac{1}{2}} \frac{E'}{E}\frac{mc}{|\vec{q}|} XJ(Q)$$

p_z – Projection of electron's momentum in scatter direction

$|\vec{q}|$ – Momentum transferred to electron

X – IA X-factor (A function of p_z, E_c, E and $\cos\theta$)

$J(Q)$ – Compton profile as a function of wavelength separation from Compton line

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MODELING COMPTON SCATTERING

<u>Sampling Method</u>: Recast DDCS into a DCS related to Klein-Nishina with new rejection and momentum sampling

$$\sigma_i d\Omega dp_z = S_i \frac{X_{KN} d(\cos\theta)}{\int_{-1}^{1} X_{KN} d(\cos\theta)} \frac{J_i\left(p_z\right) F \Theta\left(p_i - p_z\right) dp_z}{\int_{-\infty}^{p_i} J_i\left(p_z\right) F dp_z}$$

Incoherent Scattering Function

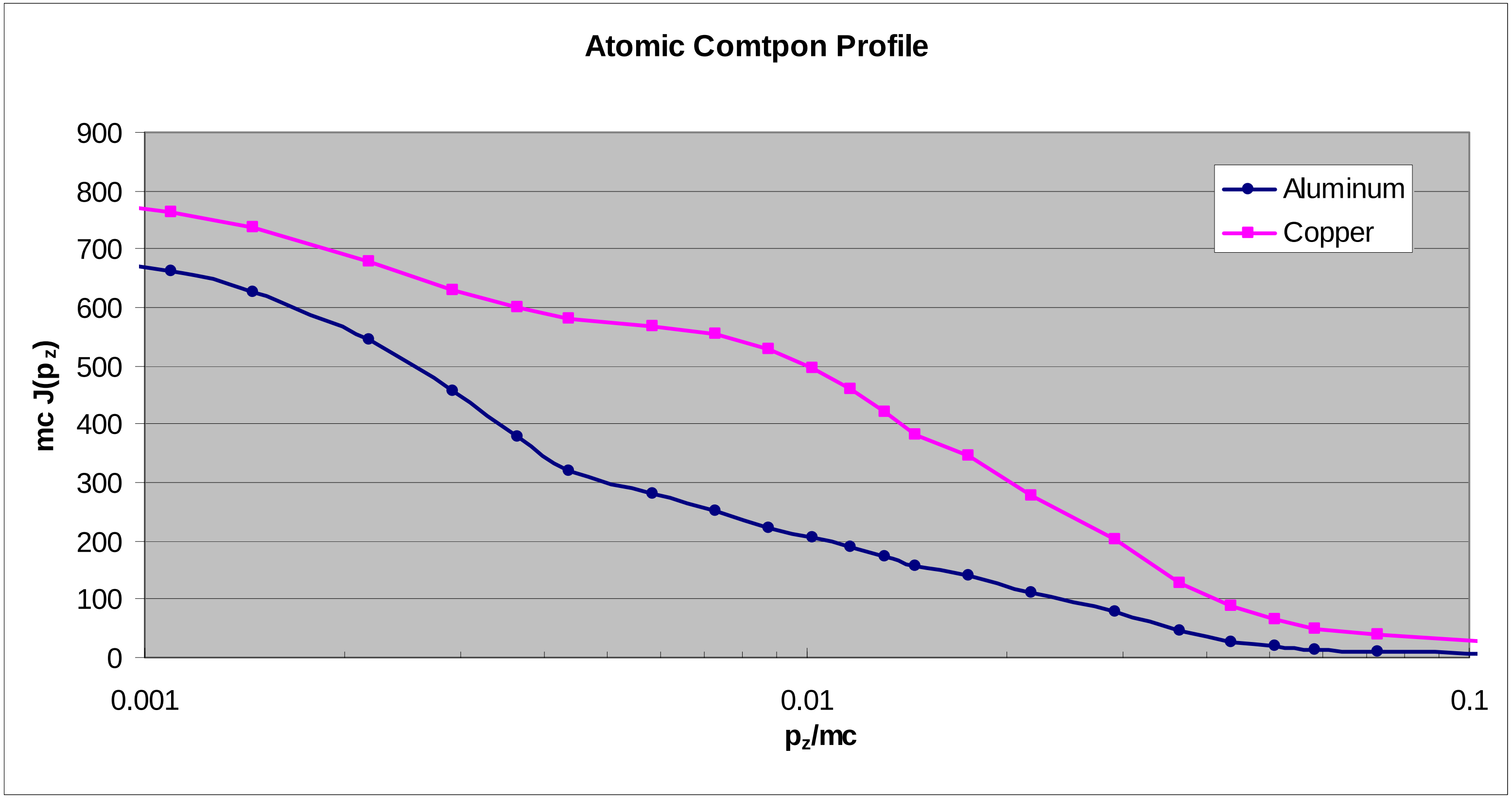
$$S_i \approx Z_i \int_{-\infty}^{p_i} J_i\left(p_z\right)\Theta\left(E - U_i\right) dp_z$$

Rejection Function of Doppler Parameter

$$F\left(p_z\right) \approx 1 + \frac{cq_c}{E}\left(1 + \frac{E_c\left(E_c - E\cos\theta\right)}{\left(cq_c\right)^2}\right)\left(\frac{p_z}{mc}\right)$$

MODELING COMPTON SCATTERING

Brusa Parameterization: Approximate $J_i(p_z)$ in such a way as to permit analytic solutions to find S_i and p_z



MODELING COMPTON SCATTERING

Brusa Parameterization:

$$J_i\left(p_z\right) \approx J_{i,0}\sqrt{2}\left(\sqrt{\frac{1}{2}}+\sqrt{2}J_{i,0}\left|p_z\right|\right)\exp\left[\frac{1}{2}-\left(\sqrt{\frac{1}{2}}+\sqrt{2}J_{i,0}\left|p_z\right|\right)^2\right]$$

Exact Expression:

$$J_i\left(p_z\right) = \iint\left|\psi\left(\vec{p}\right)\right|dp_x dp_y$$

The value of S_i represents the number of electrons in the i^{th} shell that can be effectively excited in a Compton interaction, thus the integral of a Compton profile of an orbital must be normalized

COMPTON SCATTERING ALGORITHM

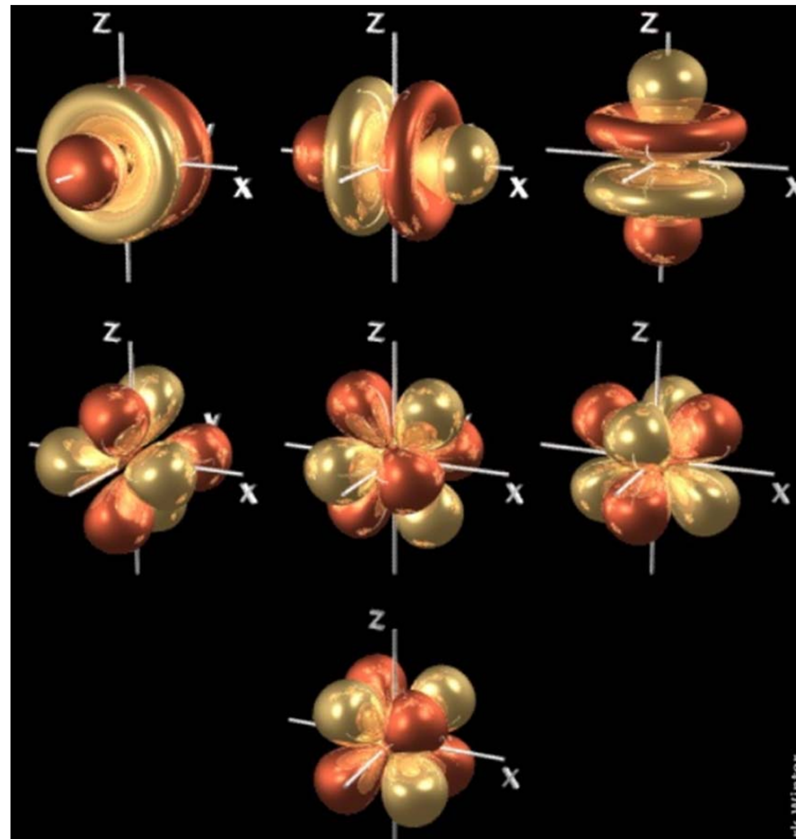
- Select shell by occupancy
  - Reject on U_i
- Sample $\cos\theta$
  - Calculate Compton details
  - Reject on S_i
- Sample p_z as a
  - Reject if less than –mc
  - Reject on $F(p_{max})$
- Deliver photon energy
  - Calculate electron's energy, cosine
  - Relax orbital vacancy by Auger and fluorescence

$$P_1(\cos\theta) = \frac{X_{\mathrm{KN}}(\cos\theta)\ \mathrm{d}\cos\theta}{\int_{-1}^{1} X_{\mathrm{KN}}(\cos\theta)\mathrm{d}\cos\theta}$$

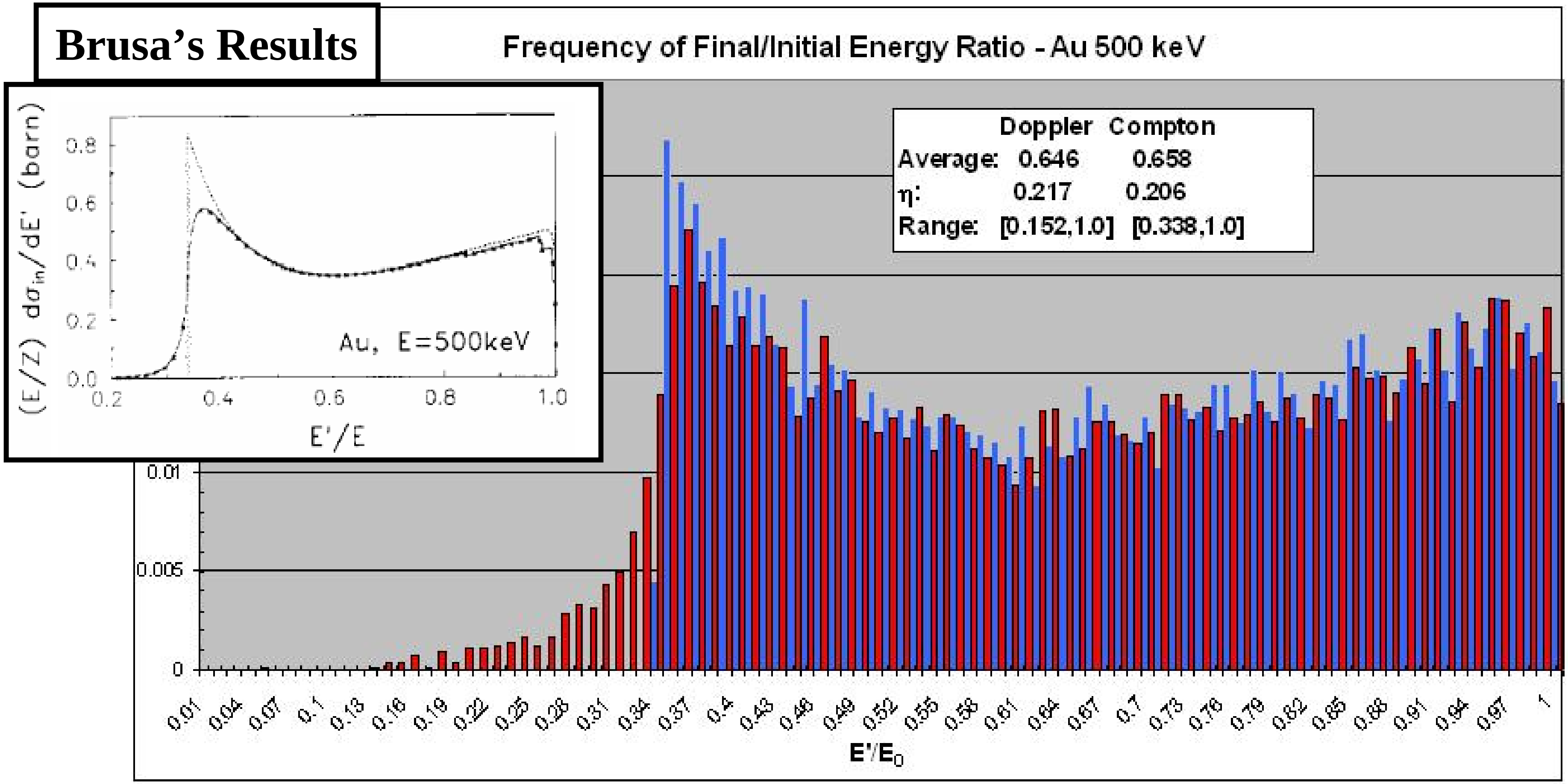
$$P_2(p_z) = \frac{J_i(p_z)F(k,\cos\theta,p_z)\Theta(p_i - p_z)\mathrm{d}p_z}{\int_{-\infty}^{p_i} \mathrm{d}p_z J_i(p_z)F(k,\cos\theta,p_z)}$$

COMPTON SCATTERING ALGORITHM

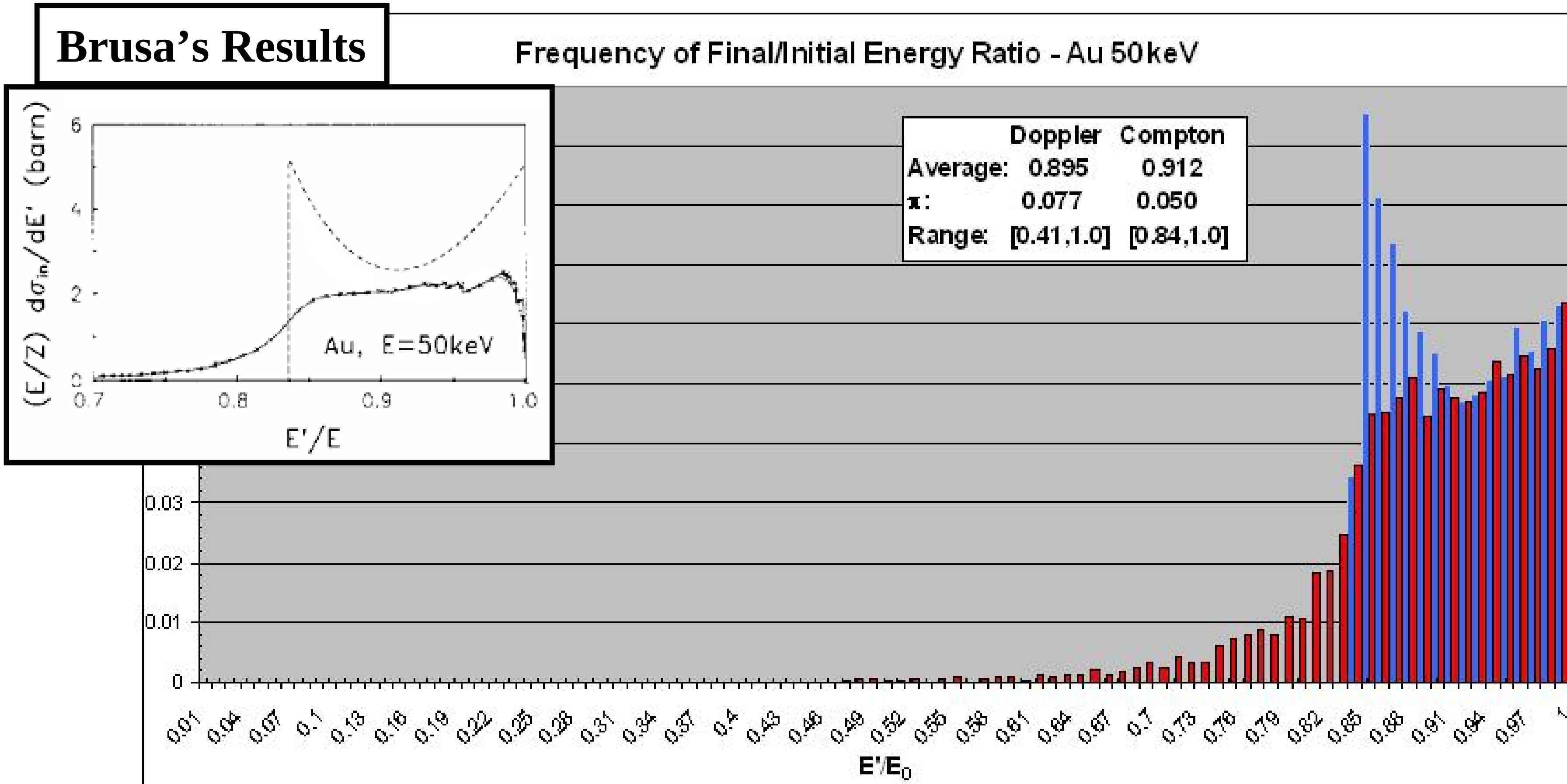
- **Shell selection is now important!**
  - **Determines binding energy (rejection occurs on this value)**
  - **Determines initial Compton profile**
- **Two types of shells exist in the data set:**
  - **Z<36 s,p,d,f orbital data**
  - **Z>36 relativistic Dirac shell formulation**



RESULTS

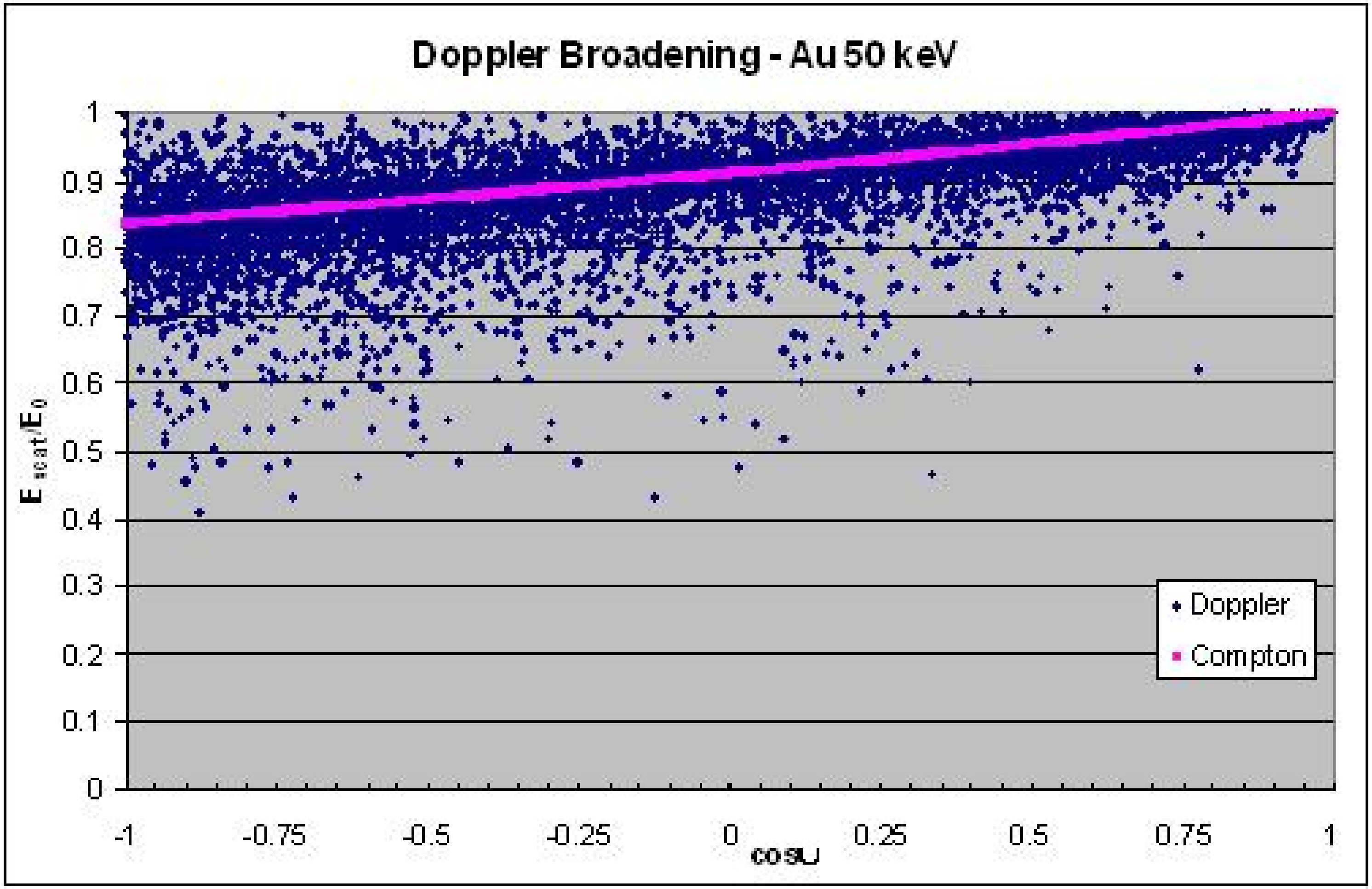

Brusa's Results
(E/Z) dσin/dE' (barn)
Au, E=500keV
E'/E
Frequency of Final/Initial Energy Ratio - Au 500 keV
Doppler Compton
Average: 0.646 0.658
η: 0.217 0.206
Range: [0.152,1.0] [0.338,1.0]
E'/E0

RESULTS



Brusa's Results
(E/Z) dσ_in/dE' (barn)
Au, E=50keV
E'/E
Frequency of Final/Initial Energy Ratio - Au 50keV
Doppler Compton
Average: 0.895 0.912
σ: 0.077 0.050
Range: [0.41,1.0] [0.84,1.0]
E'/E0

RESULTS



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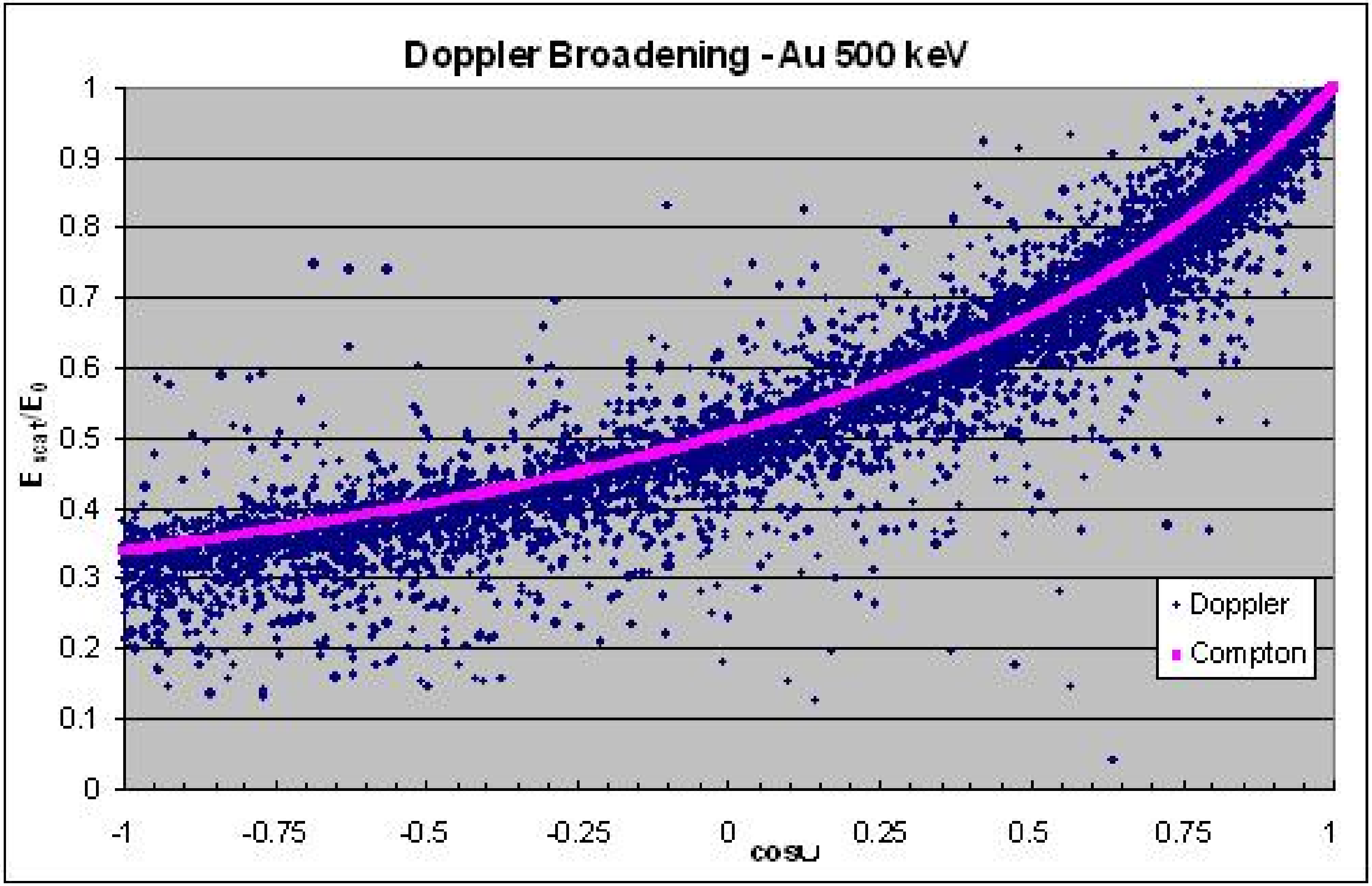
RESULTS



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RESULTS

Performance: Average Random Numbers Generated Per Compton Event

Energy	Al (Z=13)	Au (Z=79)
5 keV	12 +/- 9	17 +/- 12
50 keV	7.5 +/- 3	9.2 +/- 6
500 keV	8.0 +/- 3	8.6 +/- 5

FUTURE WORK

- Extend testing
  - Run more histories
  - Extract/compare integrated cross sections
  - Recreate experimental results
- Multiple materials
- Parallelization
- Adjoint capabilities

CONCLUSIONS

Accounting for Doppler broadening and atomic binding effects will be a user option in future versions of ITS. The sampling change in Compton scattering can be summarized as follows:

Current ITS Implementation

$$\frac{d\sigma}{d\Omega} = X_{KN} S_{WH}$$

Doppler Broadening

$$\frac{d\sigma}{d\Omega} = X_{KN} \sum_i Z_i J_i \left(p_z \right) F \Theta \left(E - E' - U_i \right)$$