MULTIPLE SCATTERING OF PHOTONS USING THE BOLTZMANN TRANSPORT EQUATION

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INTRODUCTION
MULTIPLE SCATTERING

• X-rays penetrate deeply into the matter, and, in a thick medium, give place to a phenomenon known as **multiple scattering**.

• Multiple scattering models describe the influence of the prevailing interactions in the x-ray regime (**photoelectric effect**, **Compton scattering** and **Rayleigh scattering**).
MULTIPLE SCATTERING (cont.)

• Multiple scattering models describe the influence of the prevailing interactions in the x-ray regime (photoelectric effect, Compton scattering and Rayleigh scattering)

• The photoelectric effect itself can be considered as a ‘scattering process’
Photoelectric effect as ‘scattering’

\[ h\nu \quad \text{characteristic photon} \]

\[ K \quad L_1 \quad L_2 \quad L_3 \]

\[ \text{photoelectron} \]

\[ \text{photoelectric absorption} + \text{radiative transition} = \text{photoelectric 'scattering'} \]
PREVAILING INTERACTIONS IN THE X-RAY REGIME

PRIMARY PHOTON

COHERENT SCATTERING
  - RAYLEIGH PHOTON

INCOHERENT SCATTERING
  - COMPTON PHOTON
  - COMPTON ELECTRON

PHOTOELECTRIC EFFECT
  - CHAR. X-RAYS
  - PHOTO ELECTRON

Scattered photons
Scattered electron
DESCRIPTION OF POLARIZATION
WHY POLARIZATION?

Polarization state $\rightarrow$ wave nature of photons

By considering polarization we improve the model of photon diffusion
Without polarization photons are considered only as particles. This is a good approximation in many cases, but not for phenomena that are influenced by their wave properties.
REPRESENTATION OF POLARIZED RADIATION

Stokes parameters I,Q,U,V (having the dimension of an intensity) can specify:

- Intensity of the beam
- Degree of polarization
- Orientation of the ellipse of polarization
- Ellipticity
Polarization state definition

Four parameters:

a) The intensity (the square of the electric field)

b) The degree of polarization (the fraction of elliptically polarized beam)

c) Orientation of the polarization ellipse (angle $\chi$)

d) Ellipticity (expressed by the angle $\beta$)
STOKES’ REPRESENTATION OF POLARIZED RADIATION

Definition of STOKES PARAMETERS:

\[ Q = I \cos 2\beta \cos 2\chi \]
\[ U = I \cos 2\beta \sin 2\chi \]
\[ V = I \sin 2\beta \]

Degree of polarization:

\[ P = \left( \frac{Q^2 + U^2 + V^2}{I} \right)^{1/2} \]
EXAMPLES OF THE STOKES REPRESENTATION

<table>
<thead>
<tr>
<th>Polarisation state</th>
<th>Set S (I,Q,U,V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unpolarised</td>
<td>(1,0,0,0)</td>
</tr>
<tr>
<td>Linear (generic)</td>
<td>(1,\cos2\chi,\sin2\chi,0)</td>
</tr>
<tr>
<td>Linear (</td>
<td></td>
</tr>
<tr>
<td>Linear (⊥)</td>
<td>(1,-1,0,0)</td>
</tr>
<tr>
<td>Linear (45°)</td>
<td>(1,0,1,0)</td>
</tr>
<tr>
<td>Circular</td>
<td>(1,0,0,1)</td>
</tr>
</tbody>
</table>
Modification of the polarization state due to a collision (Stokes representation)
PHYSICAL MODEL

- The photon state is changed by a matrix kernel depending on the type of the collision a. This kernel operates on the polarisation state according to the relationship:

\[
\begin{pmatrix}
I^{(n)} \\
Q^{(n)} \\
U^{(n)} \\
V^{(n)}
\end{pmatrix}
= \begin{pmatrix}
I^{(n+1)} \\
Q^{(n+1)} \\
U^{(n+1)} \\
V^{(n+1)}
\end{pmatrix}
\]
PHOTON DIFFUSION IS DESCRIBED BY A “VECTOR” TRANSPORT EQUATION (THE 1-D EQUATION IS SHOWN HERE)

\[
\eta \frac{\partial}{\partial z} \bar{f}^{(\Sigma)}(z, \bar{\omega}, \lambda) = -\mu(\lambda) \bar{f}^{(\Sigma)}(z, \bar{\omega}, \lambda) \\
+ \int d\omega' \int d\lambda' U(z) H^{(\Sigma)}(\bar{\omega}, \lambda, \bar{\omega}', \lambda') \bar{f}^{(\Sigma)}(z, \bar{\omega}', \lambda') \\
+ \delta(z) \bar{f}^{(\Sigma)}(\bar{\omega}, \lambda)
\]

where

\[
\bar{f} = \begin{bmatrix}
I(z, \bar{\omega}, \lambda) \\
Q(z, \bar{\omega}, \lambda) \\
U(z, \bar{\omega}, \lambda) \\
V(z, \bar{\omega}, \lambda)
\end{bmatrix}
\]
VECTOR TRANSPORT EQUATION (CONT.)

where

\[ H^{(S)}(\varphi, \lambda, \varphi', \lambda') = L^{(S)}(\pi - \Psi) K^{(S)}(\varphi, \lambda, \varphi', \lambda') L^{(S)}(-\Psi) \]

\[ H^{(S)} = \text{kernel matrix in the meridian plane of reference} \]

\[ K^{(S)} = \text{scattering matrix in the scattering plane of reference} \]
PHOTON DIFFUSION IS DESCRIBED BY A “VECTOR” TRANSPORT EQUATION (THE 1-D EQUATION IS SHOWN HERE)

\[ \eta \frac{\partial}{\partial z} \bar{f}(z, \omega, \lambda) = -\mu(\lambda) \bar{f}(z, \omega, \lambda) + \]

\[ \int_{0}^{\infty} d\lambda' \int_{\frac{4\pi}{4\pi}} d\omega' U(z) \bar{H}(\omega, \lambda, \omega', \lambda') \bar{f}(z, \omega', \lambda') + \delta(z) \bar{S}(\omega, \lambda) \]

where \( \bar{f} = \)

\[
\begin{bmatrix}
I(z, \omega, \lambda) \\
Q(z, \omega, \lambda) \\
U(z, \omega, \lambda) \\
V(z, \omega, \lambda)
\end{bmatrix}
\]
VECTOR TRANSPORT EQUATION (CONT.)

where

\[
\begin{aligned}
\Psi - \Psi &= \lambda, \\
\Pi - \Pi' &= \lambda',
\end{aligned}
\]

\[
\mathbf{H}(\omega, \lambda, \omega', \lambda') =
\]

\[
\mathbf{L}(\pi - \Psi) \mathbf{K}(\omega, \lambda, \omega', \lambda') \mathbf{L}(-\Psi)
\]

\[\mathbf{H} = \text{kernel matrix in the meridian plane of reference}\]

\[\mathbf{K} = \text{scattering matrix in the scattering plane of reference}\]
IMPORTANT PROPERTIES OF THE “VECTOR” TRANSPORT EQUATION

- Describes the evolution of the full polarization state (not only the intensity of the beam)
- Is linear (for the Stokes representation)
- Requires the simultaneous solution of the whole set of transport equations
- Cannot be transformed into a scalar equation!! (due to the coupling in the scattering term)
THEORETICAL MODELS
MODELS

Different degrees of approximation to describe the diffusion photons:

- **scalar model**: photons never modify an average polarization state

- **vector model**: transport of photons starting with arbitrary polarization state
Both models follow a multiple scattering scheme

<table>
<thead>
<tr>
<th></th>
<th>Photoelectric effect</th>
<th>Rayleigh scattering</th>
<th>Compton scattering</th>
</tr>
</thead>
<tbody>
<tr>
<td>one collision</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>(P) characteristic lines (discrete)</td>
<td>(R) Rayleigh peak (discrete)</td>
<td>(C) Compton peak (continuous)</td>
</tr>
<tr>
<td>two collisions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>b</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>(P,P) XRF secondary enhancement (discrete on XRF line)</td>
<td>(P,R) XRF enhancement due to scattering (discrete on XRF line)</td>
<td>(P,C) XRF enhancement due to scattering (continuous on XRF line)</td>
</tr>
<tr>
<td></td>
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<tr>
<td></td>
<td>(R,P) XRF enhancement due to scattering (discrete on XRF line)</td>
<td>(R,R) second order scattering (discrete on Rayleigh peak)</td>
<td>(R,C) second order scattering (continuous on Compton peak)</td>
</tr>
<tr>
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<tr>
<td></td>
<td>(C,P) XRF enhancement due to scattering (discrete on XRF line)</td>
<td>(C,R) second order scattering (continuous on Compton peak)</td>
<td>(C,C) second order scattering (continuous on Compton peak)</td>
</tr>
</tbody>
</table>
Scalar transport equation

\[ I = \sum_i I^{(i)} \]

SCALAR EQUATION
Vector transport equation

\[ I = \Sigma_i I^{(i)} \]
LET US SHOW TWO SIMPLE EXAMPLES

1) Scattering of unpolarized radiation
2) Scattering of linearly polarized radiation
1) Unpolarized Rayleigh scattering
How scattering polarizes a beam

Unpolarized beam

Scatterer

90 degrees scattering
Unpolarized beam (composed by rays with electric vector randomly oriented around the propagation direction)

After scattering the beam is partially (totally) polarized depending on the type of interaction and the scattering geometry
2) Polarized Rayleigh scattering

Electric vector parallel to the scattering plane

incident beam

right angle scattering
Summary for Linear Polarization

Linearly polarized beam with electric vector parallel to the scattering plane

Almost null scattering at 90 degrees
COMBINING BOTH PROPERTIES

Scatterer = polarizer

Almost null scattering

90 degrees scattering

90 degrees scattering

Scatterer = polarizer

Unpolarized beam
THE CODES
The transport equation is solved using an order-of-collisions scheme, yielding comparable results for deterministic and Monte Carlo solutions.
### Deterministic vs. Monte Carlo

<table>
<thead>
<tr>
<th></th>
<th>Deterministic</th>
<th>Monte Carlo (statistical)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scope of the solution</td>
<td>Global</td>
<td>Local</td>
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<tr>
<td>Accuracy</td>
<td>↑</td>
<td>↓</td>
</tr>
<tr>
<td>Capability to describe geometry</td>
<td>↓</td>
<td>↑</td>
</tr>
<tr>
<td>Number of collisions</td>
<td>↓</td>
<td>↑</td>
</tr>
<tr>
<td>Developed codes</td>
<td>SHAPE</td>
<td>MCSHAPE</td>
</tr>
</tbody>
</table>
CHARACTERISTICS OF THE CODE MCSHAPE

- Arbitrary polarization state of the source
- Multi-layer multi-component homogeneous targets
- Monochromatic or polychromatic source
- Doppler broadening (for Compton scattering)
- Full description of the polarization state
- N-collisions
The source is unpolarized and monochromatic.
The sample is carbon and the scattering angle is 90°.
• Development of two different codes:
  - MCSHAPE0: max. 4 collisions and analog calculation
  - MCSHAPE1: no limits in number of collisions
• First version: Pascal (1995)
• Present versions: 1D and 3D written in FORTRAN 90
• Platforms: Windows and LINUX
• Parallelization: MPI (under LINUX)
These codes are going to be distributed by NEA Data Bank (OECD) and RSICC (US-DOE)
## CODES COMPARISON (part 1: Physics)

<table>
<thead>
<tr>
<th>Features</th>
<th>Details</th>
<th>SHAPE v2.20</th>
<th>D3DSHAPE v1.0</th>
<th>MCSHAPE v2.50</th>
</tr>
</thead>
<tbody>
<tr>
<td>photoelectric effect</td>
<td></td>
<td>❌</td>
<td>❌</td>
<td>❌</td>
</tr>
<tr>
<td>~1000 characteristic lines</td>
<td></td>
<td>❌</td>
<td>❌</td>
<td>❌</td>
</tr>
<tr>
<td>line width</td>
<td></td>
<td>❌</td>
<td></td>
<td></td>
</tr>
<tr>
<td>atomic Rayleigh scattering</td>
<td></td>
<td>❌</td>
<td>❌</td>
<td></td>
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<tr>
<td>atomic Compton scattering</td>
<td></td>
<td>❌</td>
<td>❌</td>
<td></td>
</tr>
<tr>
<td>Compton profile</td>
<td>first collision only</td>
<td>❌</td>
<td></td>
<td>❌</td>
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<tr>
<td>electron bremsstrahlung</td>
<td>foreseen in v3</td>
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<td>open data bases</td>
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<tr>
<td>user defined elements</td>
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<tr>
<td>infinite thickness targets</td>
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<td>finite thickness targets</td>
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<tr>
<td>multilayer targets</td>
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<td>polarization representation</td>
<td>Stokes</td>
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<td><strong>source polarization state</strong></td>
<td><strong>linear/ unpolarised</strong></td>
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<td><strong>arbitrary</strong></td>
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<td>calculated spectrum</td>
<td>intensity component only</td>
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<td><strong>full polarization state</strong></td>
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<td>monochromatic source</td>
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<td>external detector</td>
<td>solid state Si/Ge</td>
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<tr>
<td>reflection geometry</td>
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<td>transmission geometry</td>
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## CODES COMPARISON (part 2: model and programming)

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<th>Features</th>
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<td></td>
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<td>1-D spatial geometry</td>
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<td>✗</td>
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<tr>
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<td>3-D spatial geometry</td>
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<td>using MCSHAPE3D</td>
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<td>Applications</td>
<td>analytical chemistry</td>
<td>✗</td>
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<td>dosimetry</td>
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<td>with MCSHAPE3D</td>
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<td>radiation transport teaching</td>
<td>✗</td>
<td>✗</td>
<td>✗</td>
</tr>
</tbody>
</table>
3D - MCSHAPE

• TARGET:
  – heterogeneus target -> VOXEL MODEL
  – interfaced with GAMBIT (FLUENT environment)

• SOURCE:
  – uniform source on a disk
  – uniform source on a rectangle
  – point source

• DETECTOR:
  – disk detector
  – rectangular detector
  – plane infinite detector
  – Collimator in front of the detector

3D – MCSHAPE: XRF Tomography

- **Total dimension:** 0.1 x 0.1 x 0.01 cm
- **Composition:**
  - Region \(A\): \(C + 0.1\% \text{Sr}, \rho = 1.0 \text{ g/cm}^3\)
  - Other elements:
    - Region \(B\): \(\text{SiO}_2 + 1\% \text{Fe}, \rho = 2.23 \text{ g/cm}^3\)
    - Region \(C\): \(\text{SiO}_2 + 1\% \text{Ba}, \rho = 2.23 \text{ g/cm}^3\)
    - Region \(D\): \(\text{SiO}_2 + 1\% \text{Zr}, \rho = 2.23 \text{ g/cm}^3\)

- **Source:**
  - Energy: 59.54 keV
  - Type: point source
  - Unpolarized

- **Detector:**
  - Type: disk with 30 mm^2 of total area
  - No collimator

3D – MCSHAPE: XRF Tomography

Full spectrum Sr Ba Zr Fe

Full spectrum Sr Ba Zr Fe

OPEN PROBLEM #1: COHERENCE

• Vector transport equation behaves linearly only for an incoherent source

• Diffusion of coherent radiation is not considered yet in transport models used to describe x-ray diffusion
OPEN PROBLEM #2: VARIANCE REDUCTION

ACTUALLY:

• Variance reduction on the angular variables is performed using the average kernel.

• The Stokes components are computed using weights.

→ MIXED METHOD
→ OPTIMIZED INTENSITY
CONCLUSIONS
CONCLUSIONS

• MCSHAPE was developed:

- to provide a full description of the polarization state evolution through multiple scattering collisions

- to extend results of the deterministic method to higher orders of collision
CONCLUSIONS

The vector MC code MCSHAPE give:

- a detailed description of multiple scattering of the prevailing interactions in the x-ray regime

- full analysis of the final state of polarization at each collision number

- for infinite or finite, and single or multi-layer multi-component targets
CONCLUSIONS cont.

• Good agreement with experimental data has been obtained for both, unpolarized and polarized sources
• More detailed tests are being planned in the future
• Experimental comparisons are welcome!!!
• As well as scientific cooperations!!!