PHOTON TRANSPORT SIMULATION, INCLUDING POLARIZATION

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DESCRIPTION OF POLARIZATION

WHY POLARIZATION?

Polarization state → wave nature of photons

By considering polarization we improve the model of photon diffusion

Without polarization photons are considered only as a particles

⬇

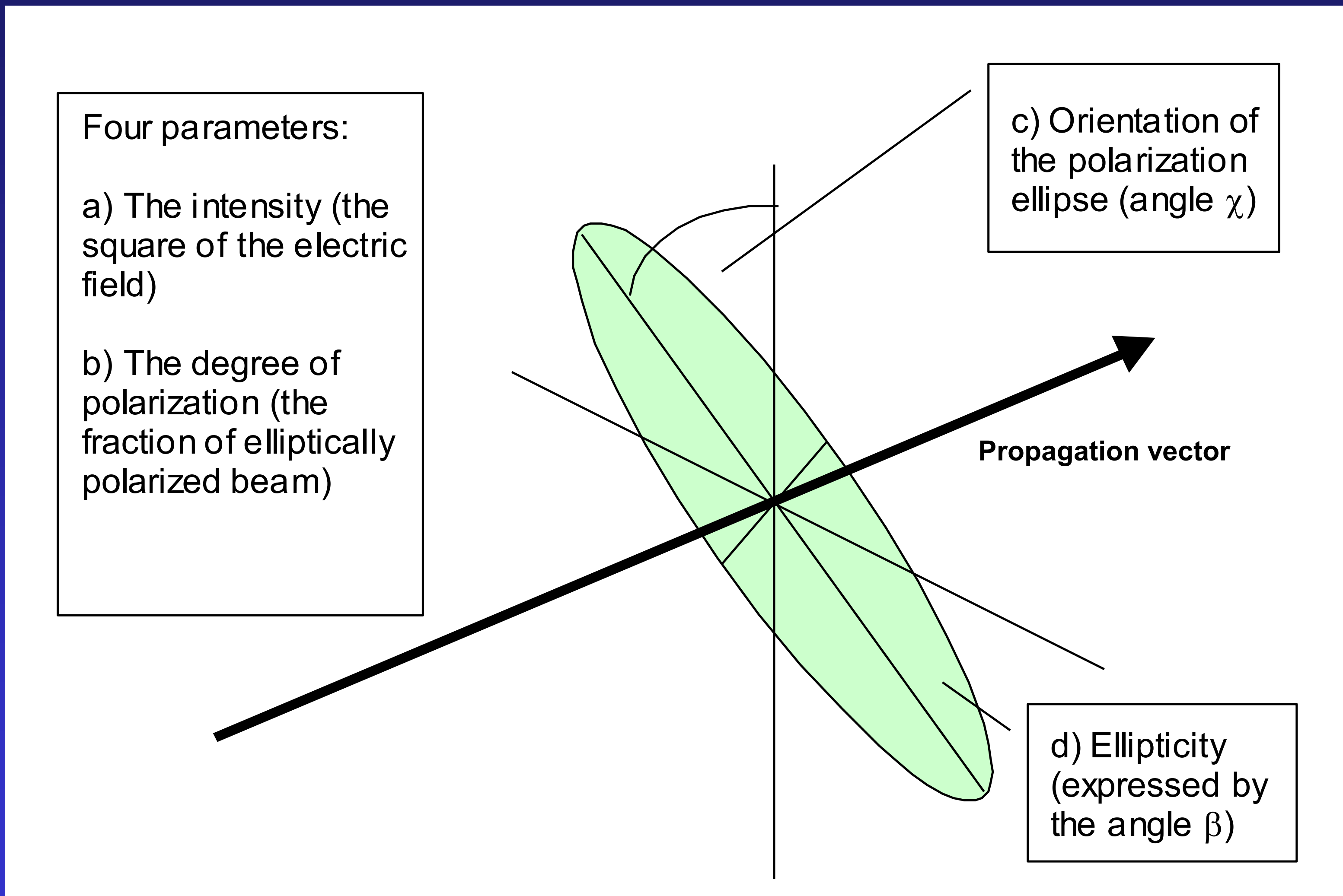
a good approximation in many cases, but not for phenomena that are influenced by their wave properties

REPRESENTATION OF POLARIZED RADIATION

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

- **Intensity of the beam**
- **Degree of polarization**
- **Orientation of the ellipse of polarization**
- **Ellipticity**

Polarization state definition



STOKES' REPRESENTATION OF POLARIZED RADIATION

Definition of STOKES PARAMETERS:

$$Q = I \cos 2\beta \cos 2\chi$$

$$U = I \cos 2\beta \sin 2\chi$$

$$V = I \sin 2\beta$$

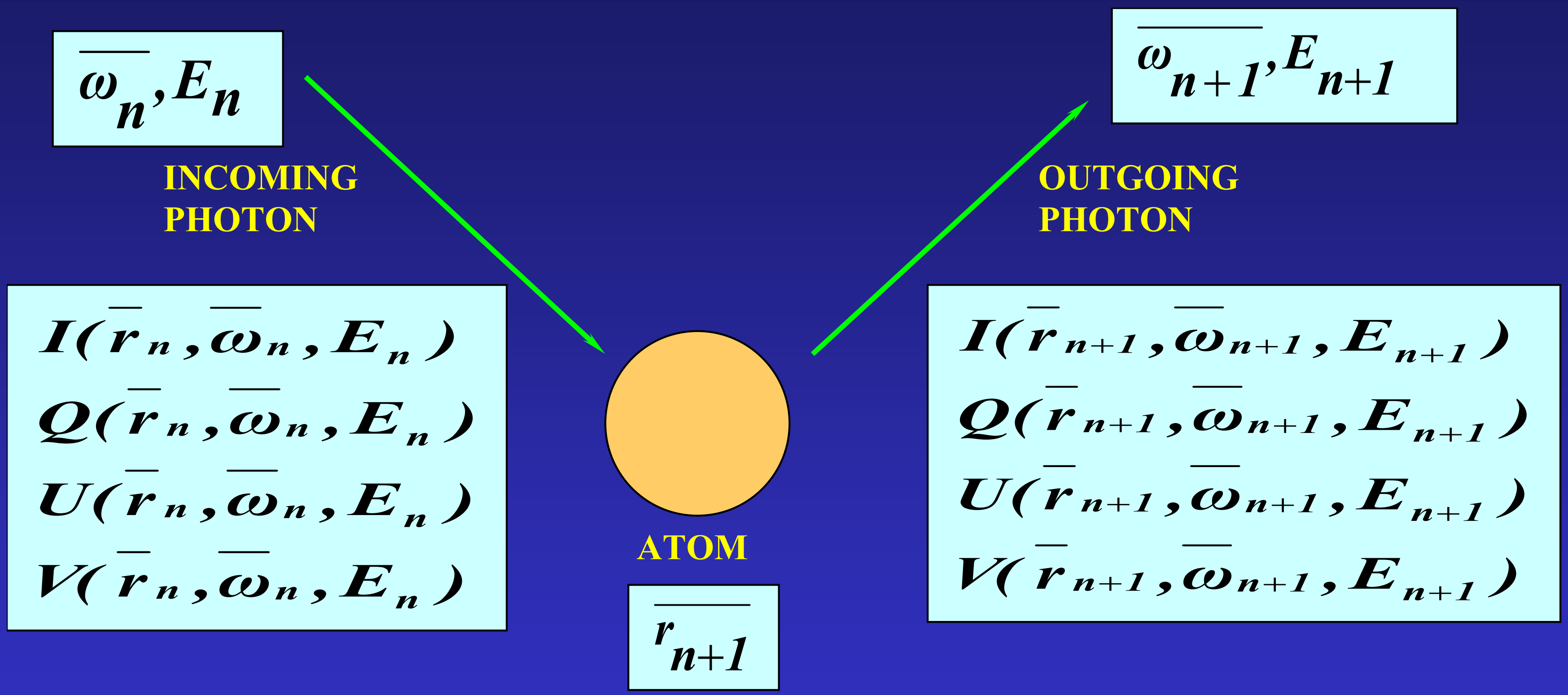
Degree of polarization:

$$P = \frac{(Q^2 + U^2 + V^2)^{1/2}}{I}$$

EXAMPLES OF THE STOKES REPRESENTATION

Polarisation state	Set S (I,Q,U,V)
Unpolarised	(1,0,0,0)
Linear (generic)	$(1,\cos 2\chi,\sin 2\chi,0)$
Linear (‖)	(1,1,0,0)
Linear (⊥)	(1,-1,0,0)
Linear (45°)	(1,0,1,0)
Circular	(1,0,0,1)

COLLISION SCHEME



Modification of the polarization state due to a collision (Stokes representation)

TWO RELEVANT ASPECTS

- A collision always changes the polarization state
- The angular distribution for scattered unpolarized and polarized photons is very different

PHOTON DIFFUSION IS DESCRIBED BY A "VECTOR" TRANSPORT EQUATION (THE 1-D EQUATION IS SHOWN HERE)

$$\eta \frac{\partial}{\partial z} \vec{f}^{(S)}(z, \vec{\varpi}, \lambda) = -\mu(\lambda)\vec{f}^{(S)}(z, \vec{\varpi}, \lambda) + \int_{4\pi} d\varpi' \int_0^{\infty} d\lambda' \mathrm{U}(z)\mathrm{H}^{(S)}(\vec{\varpi}, \lambda, \vec{\varpi}', \lambda')\vec{f}^{(S)}(z, \vec{\varpi}', \lambda') + \delta(z)\vec{S}^{(S)}(\vec{\varpi}, \lambda)$$

where

$$\overline{f} = \begin{bmatrix} I(z, \overline{\omega}, \lambda) \\ Q(z, \overline{\omega}, \lambda) \\ U(z, \overline{\omega}, \lambda) \\ V(z, \overline{\omega}, \lambda) \end{bmatrix}$$

VECTOR TRANSPORT EQUATION (CONT.)

where

$$H^{(S)}(\vec{\varpi}, \lambda, \vec{\varpi}', \lambda') = L^{(S)}(\pi - \Psi) K^{(S)}(\vec{\varpi}, \lambda, \vec{\varpi}', \lambda') L^{(S)}(-\Psi')$$

$H^{(S)}$ = kernel matrix in the meridian plane of reference

$K^{(S)}$ = 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 in 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

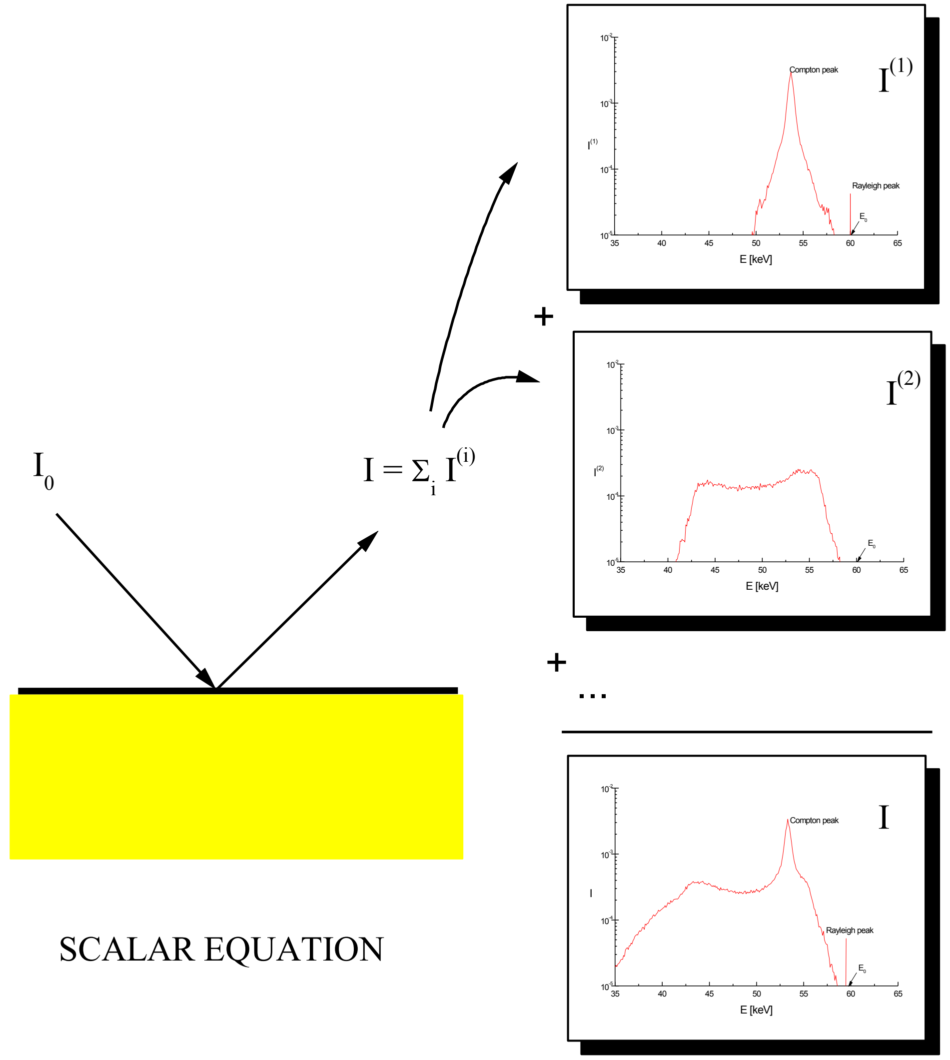
one collision

a	Photoelectric effect	Rayleigh scattering	Compton scattering
	(P) characteristic lines (discrete)	(R) Rayleigh peak (discrete)	(C) Compton peak (continuous)

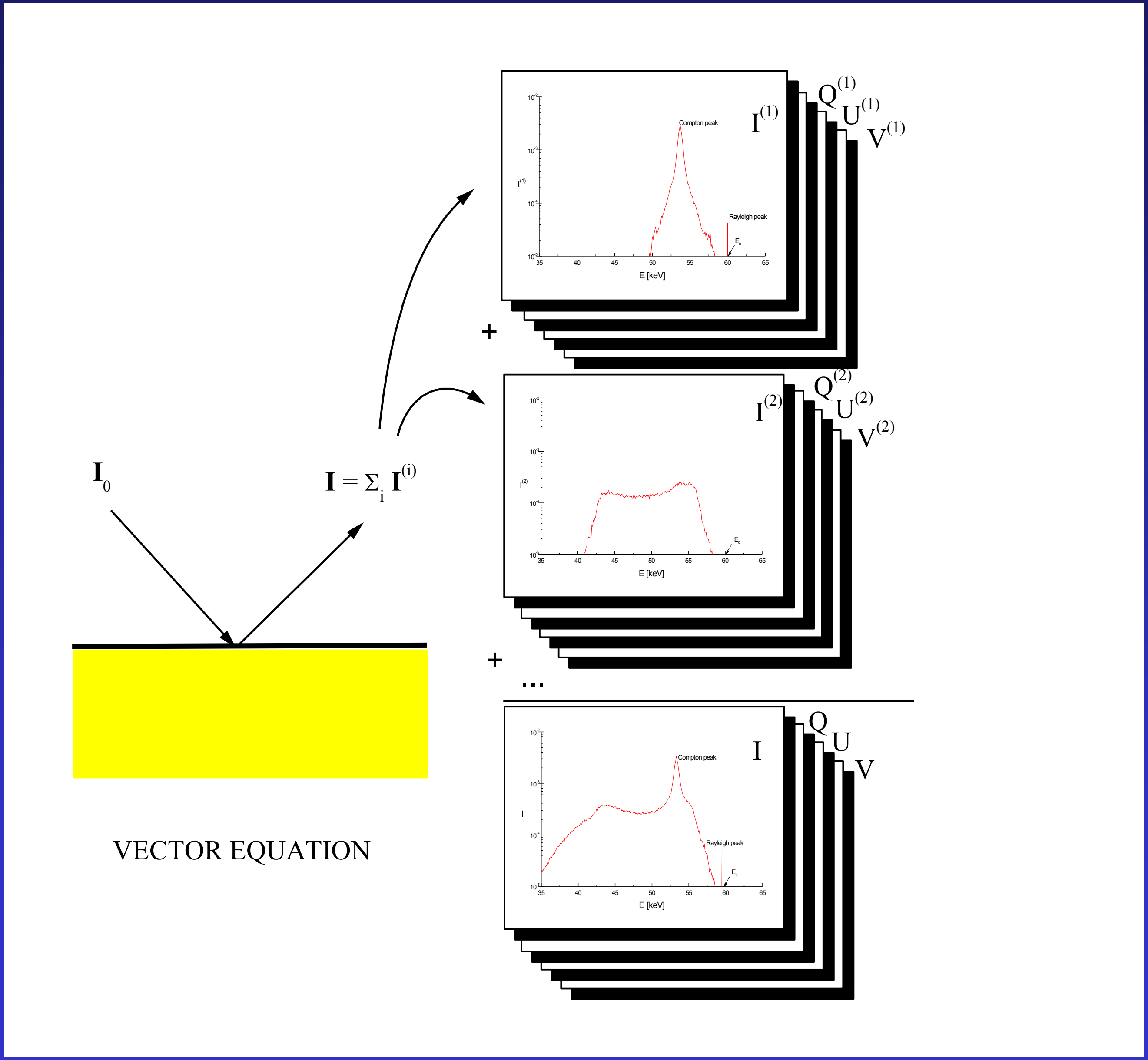
two collisions

a \ b	Photoelectric effect	Rayleigh scattering	Compton scattering
Photoelectric effect	(P,P) XRF secondary enhancement (discrete on XRF line)	(P,R) XRF enhancement due to scattering (discrete on XRF line)	(P,C) XRF enhancement due to scattering (continuous on XRF line)
Rayleigh scattering	(R,P) XRF enhancement due to scattering (discrete on XRF line)	(R,R) second order scattering (discrete on Rayleigh peak)	(R,C) second order scattering (continuous on Compton peak)
Compton scattering	(C,P) XRF enhancement due to scattering (discrete on XRF line)	(C,R) second order scattering (continuous on Compton peak)	(C,C) second order scattering (continuous on Compton peak)

Scalar transport equation



Vector transport equation

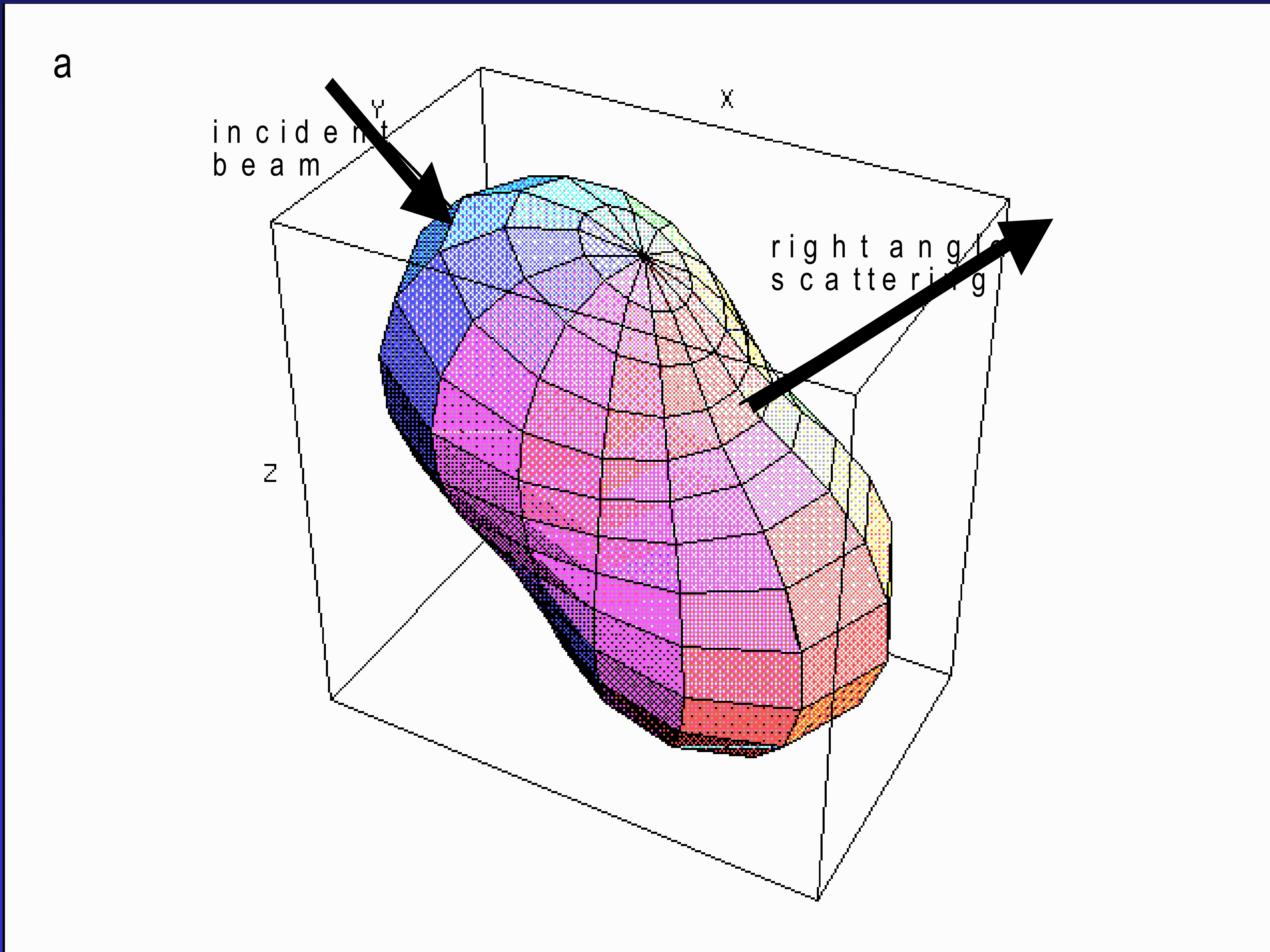


EXAMPLES

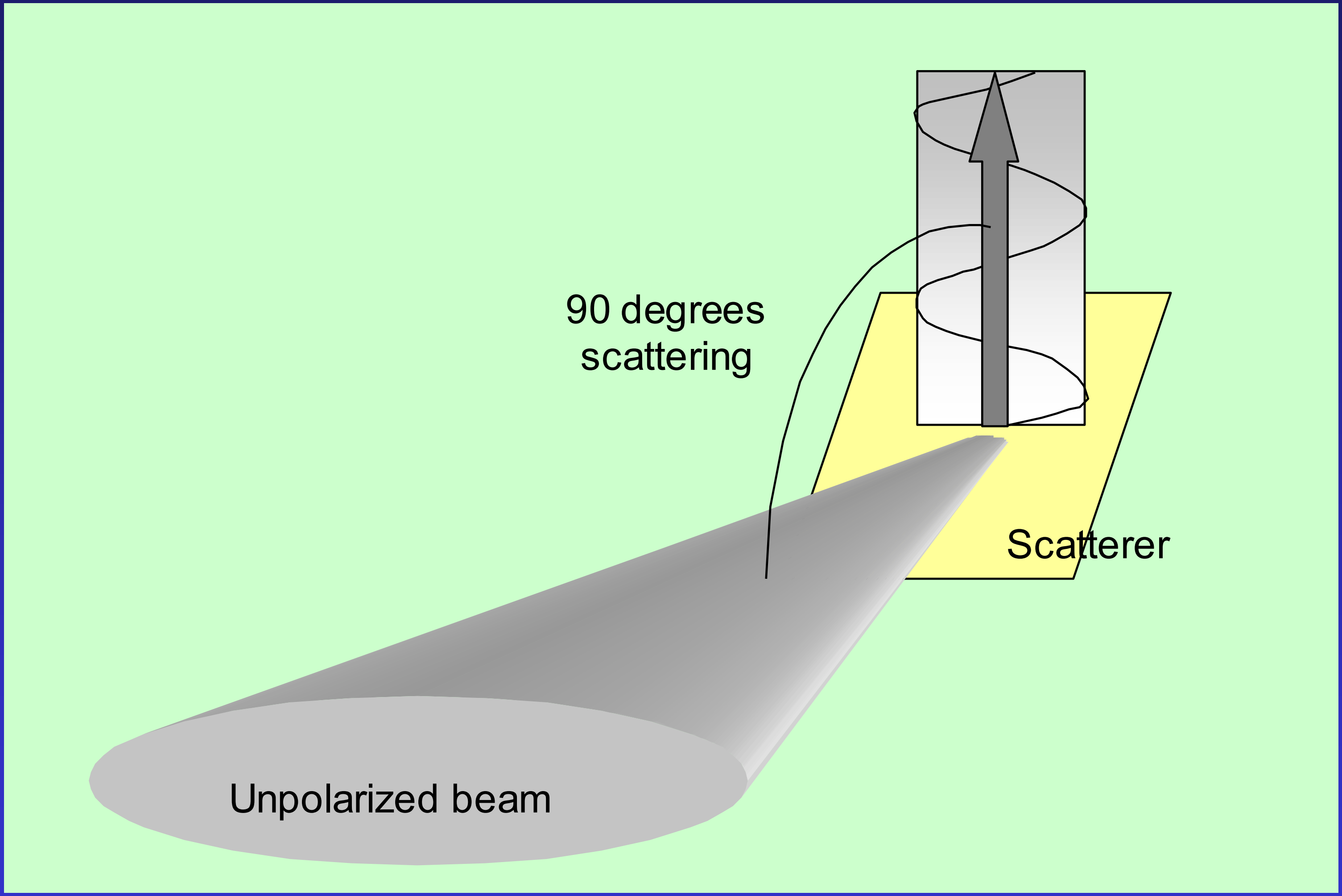
LET US SHOW TWO SIMPLE EXAMPLES

1) Scattering of unpolarized radiation
2) Scattering of linearly polarized radiation

1) Unpolarized Rayleigh scattering



How scattering polarizes a beam



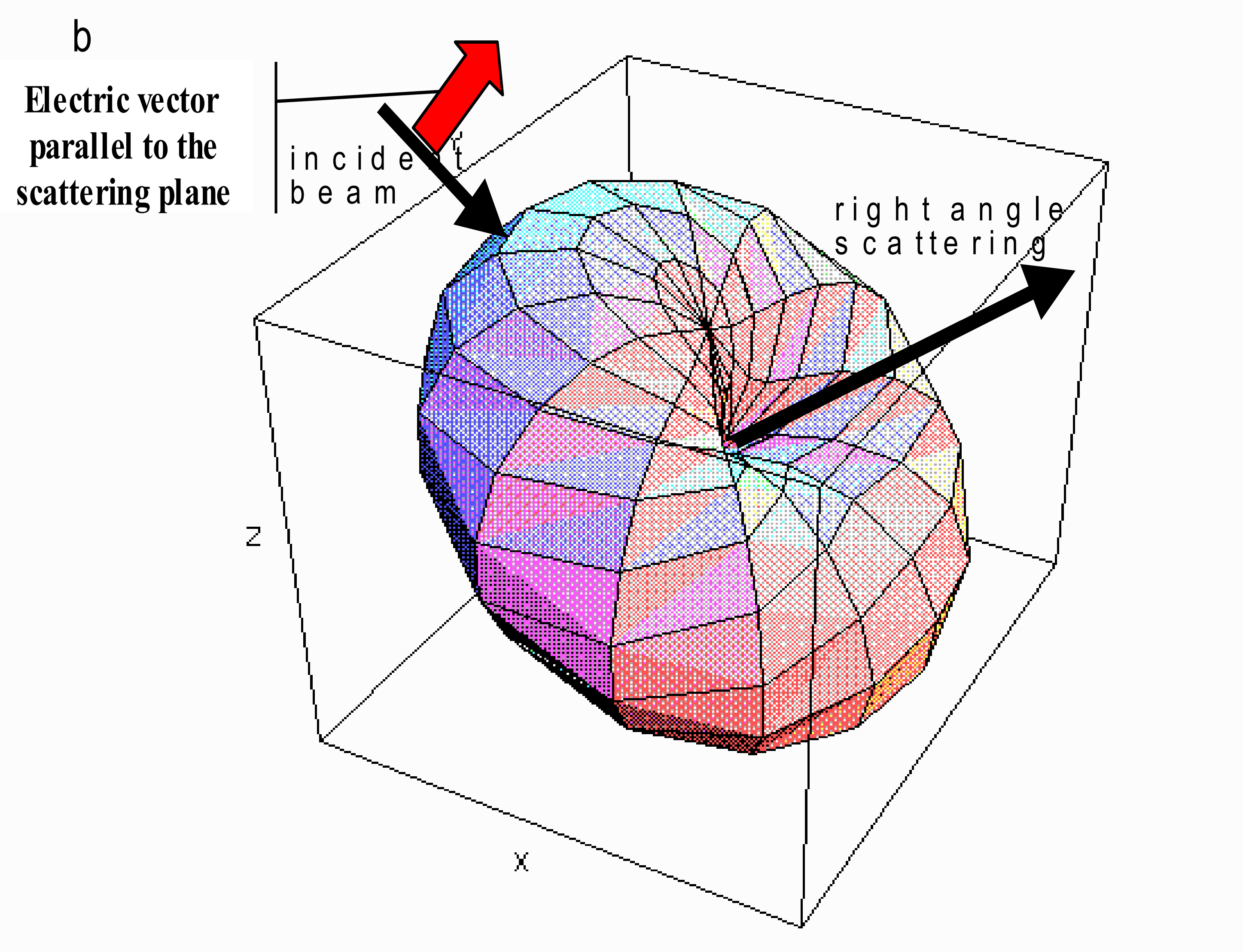
EFECTS ON UNPOLARIZED RADIATION (SUMMARY)

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

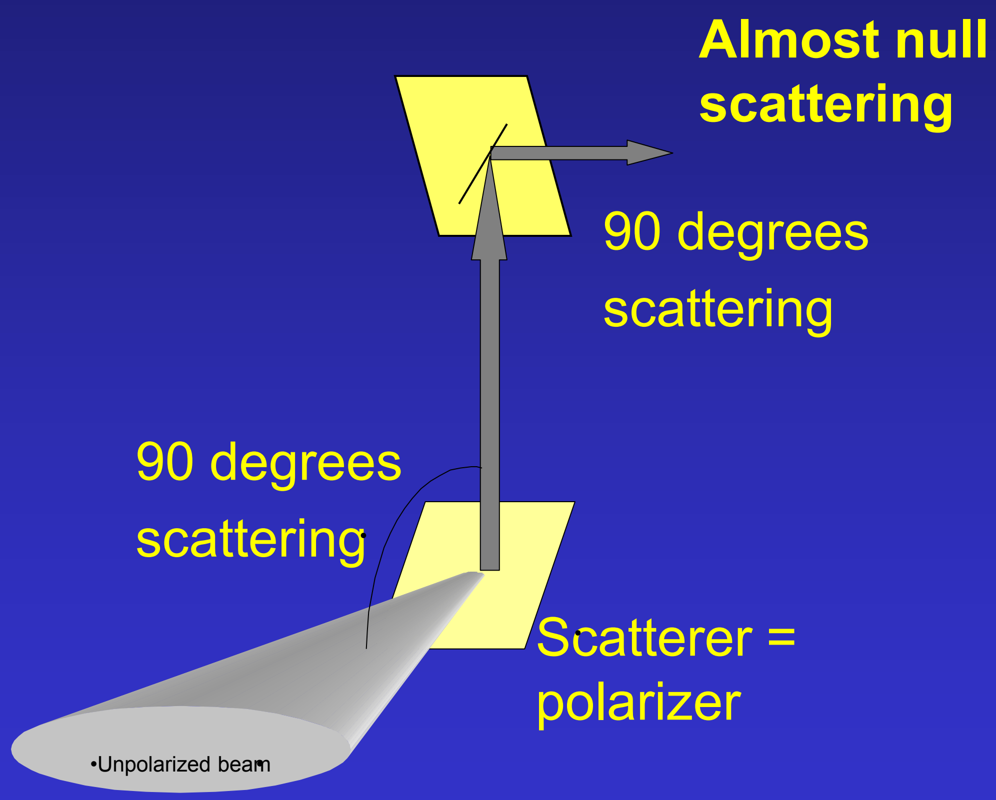
2) Polarized Rayleigh scattering



SUMMARY FOR LINEAR POLARIZATION

Linearly polarized beam with electric vector parallel to the scattering plane ➡ **Almost null scattering at 90 degrees**

COMBINING BOTH PROPERTIES



THE CODES

SOLUTION TECHNIQUES

The transport equation is solved using an order-of-collisions scheme

↓

comparable results for deterministic and Monte Carlo solutions

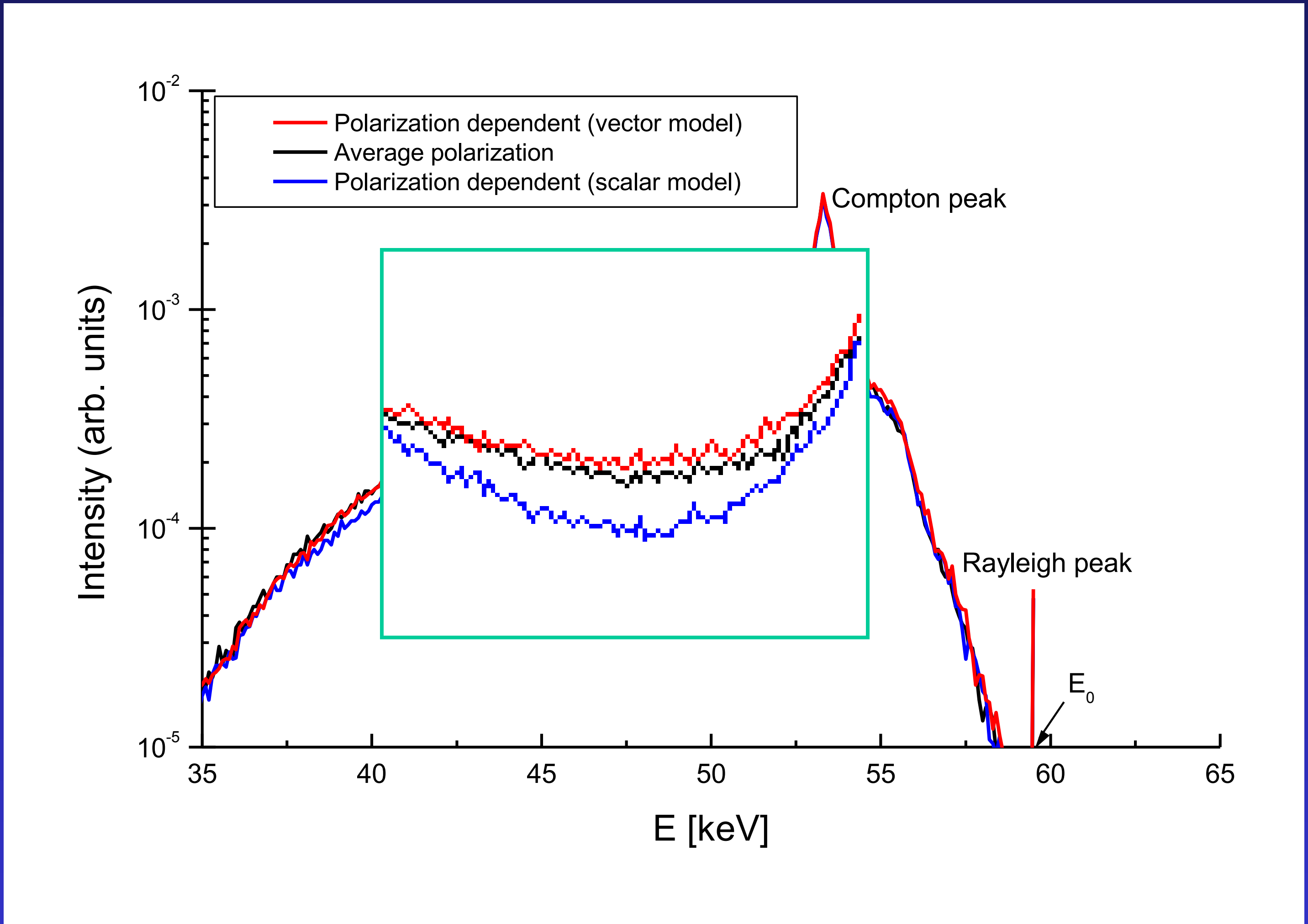
Deterministic vs. Monte Carlo

Solution	Deterministic	Monte Carlo (statistical)
Scope of the solution	Global	Local
Accuracy	↑	↓
Capability to describe the geometry	↓	↑
Number of collisions	↓	↑
Developed codes	SHAPE	MCSHAPE

CHARACTERISTICS OF THE CODE MCSHAPE

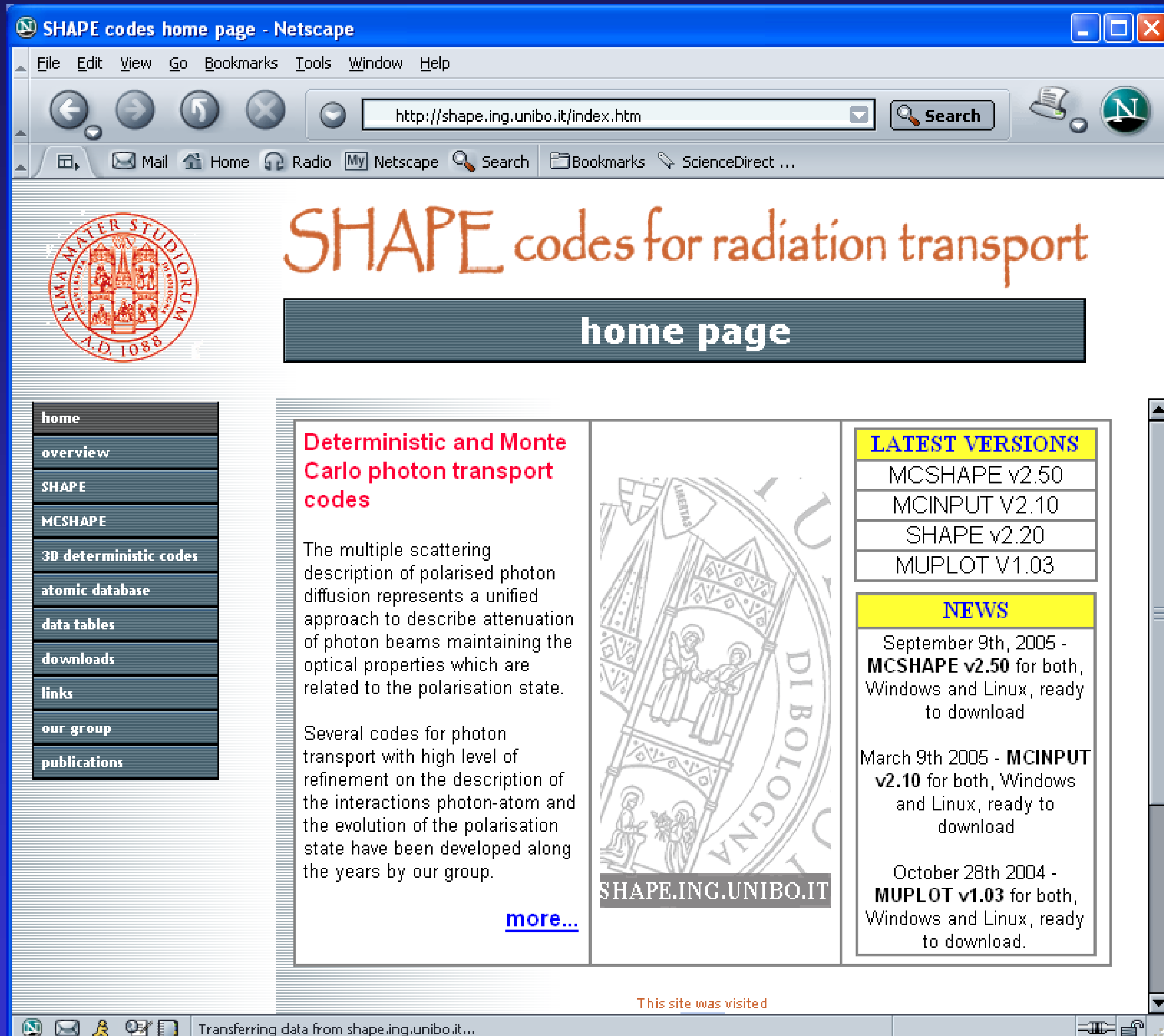
- Photon transport
- Arbitrary polarization state of the source
- Multi-layer multi-component homogeneous targets
- Monochromatic or polychromatic source
- Doppler broadening (for Compton scattering)
- Full description of the polarization state
- N-collisions
- 1D and 3D versions

COMPARISON WITH SCALAR VERSION



The source is unpolarized and monochromatic.
The sample is carbon and and the scattering angle is 90°.

WEB SITE http://shape.ing.unibo.it



These codes are going to be distributed by NEA Data Bank (OECD) and RSICC (US-DOE)

CODES COMPARISON (part 1: Physics)

Features	Details	SHAPE v2.20	D3DSHAPE v1.0	MCSHAPE v2.61
Physics	photoelectric effect	☒	☒	☒
	~1000 characteristic lines	☒	☒	☒
	line width	☒		☒
	atomic Rayleigh scattering	☒	☒	☒
	atomic Compton scattering	☒	☒	☒
	Compton profile	first collision only	☒	☒
	electron bremsstrahlung	foreseen in v3	☒	foreseen in v3
	open data bases	☒	☒	☒
	user defined elements			foreseen in v3
	infinite thickness targets	☒	☒	☒
	finite thickness targets		☒	☒
	multilayer targets			☒
	polarization representation	Stokes		Stokes
	source polarization state	**linear/ unpolarised**	unpolarised	**arbitrary**
	calculated spectrum	intensity component only		**full polarization state**
	monochromatic source	☒	☒	☒
	polychromatic source	postprocessor		☒
	external detector	solid state Si/Ge		foreseen in v3
	reflection geometry	☒	☒	☒
	transmission geometry			☒

UNIQUE FEATURES!

CODES COMPARISON (part 2: model and programming)

Features	Details	SHAPE v2.20	D3DSHAPE v1.0	MCSHAPE v2.61
Miscellaneous	Detector response	Ge and Si 1 collision escape only photoelectric		**arbitrary detector** **N-collisions escape** **all interactions**
	selective computation of single interaction chains	☒	partial	partial
Transport model	particle	photons	photons / electrons	photons
	scalar equation	☒	☒	
	vector equation	☒		☒
	solution	deterministic	deterministic	Monte Carlo
	collisions	3	3	100
	1-D spatial geometry	☒		☒
	3-D spatial geometry		☒	**using MCSHAPE3D**
Code	language	DELPHI	FORTRAN 77	FORTRAN 90
	additional libraries	graphics		WINTERACTER
	platform	WINDOWS	LINUX	WINDOWS / LINUX
	distribution	web site	alpha testing	web site
	parallelization			MPICH v1.0 (only Linux)
Applications	spectroscopy	☒	☒	☒
	analytical chemistry	☒	☒	☒
	radiation metrology	☒	☒	☒
	x-ray optics			with MCSHAPE3D
	dosimetry		foreseen in v2	with MCSHAPE3D
	radiation transport teaching	☒	☒	☒

NEW!!
Version 2.61

NEW!!
3D version of MCSHAPE

3D - MCSHAPE

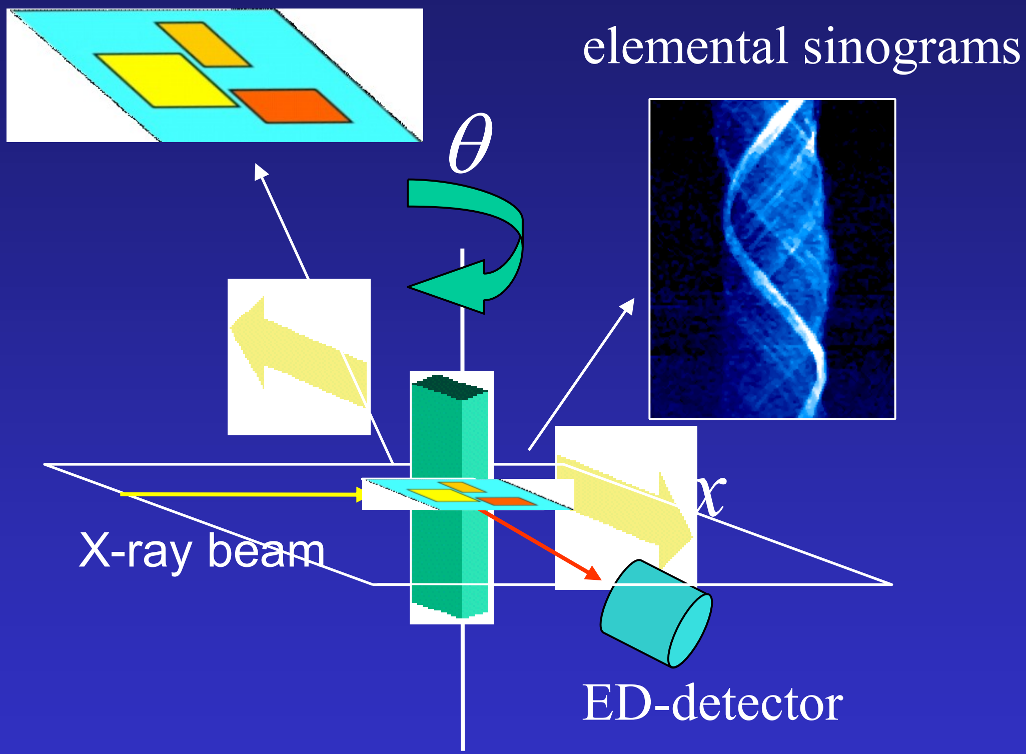
- TARGET:
  - heterogeneus target -> *VOXEL MODEL*
  - interfaced with GAMBIT (FLUENT environment)

- 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

V. Scot, J.E. Fernandez, L. Vincze, K. Janssens, submitted to NIM-B (2005)

3D – MCSHAPE: XRF Tomography



- **Total dimension**: 0.1 x 0.1 x 0.01 cm
- **Composition**:

  Region **A**: **C + 0.1%Sr**, ρ = 1.0 g/cm^3

  Other elements:

  Region **B**: **SiO_2 + 1%Fe**, ρ = 2.23 g/cm^3

  Region **C**: **SiO_2 + 1%Ba**, ρ = 2.23 g/cm^3

  Region **D**: **SiO_2 + 1%Zr**, ρ = 2.23 g/cm^3

- **Source**:

  energy: 59.54 keV

  type: point source

  unpolarized

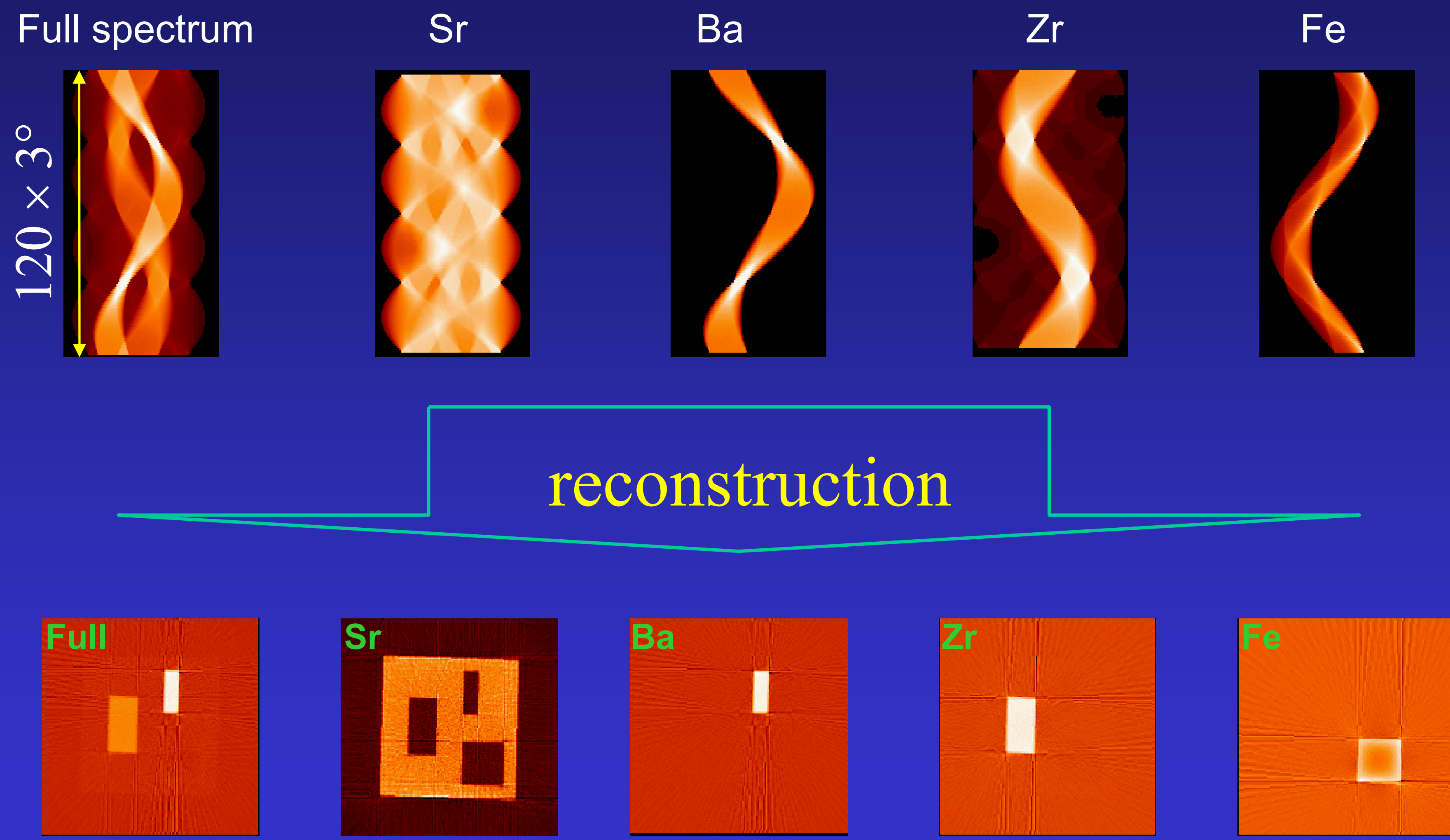
- **Detector**:

  type: disk with 30 mm^2 of total area

  no collimator

V. Scot, J.E. Fernandez, L. Vincze, K. Janssens, NIM-B 263 (2005) 204

3D – MCSHAPE: XRF Tomography



V. Scot, J.E. Fernandez, L. Vincze, K. Janssens, NIM-B 263 (2007) 204

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

The vector transport equation for photons (Boltzmann-Chandrasekhar) :

- provides a full description of the polarization state evolution through multiple scattering collisions
- provides a correct picture of the radiation field (uses the proper angular distribution)

CONCLUSIONS (cont.)

The vector code MCSHAPE:

- provides a **detailed description of multiple scattering** for the prevailing interactions in the x-ray regime (for **infinite or finite**, and **single or multi-layer multi-component targets** and recently **3D targets**)
- gives a **full analysis of the final state of polarization** at each collision number
- extends the results of the deterministic method to **higher orders of collision and arbitrary geometries**

CONCLUSIONS (cont.)

- Good agreement with experimental data has been obtained for both, unpolarized and polarized sources

- Foreseen applications in several fields:
  - x- or γ-ray tomography,
  - x- or γ-ray dosimetry,
  - solution of the inverse problem using the adjoint trasport equation.