



THE DETERMINISTIC CODE SHAPE

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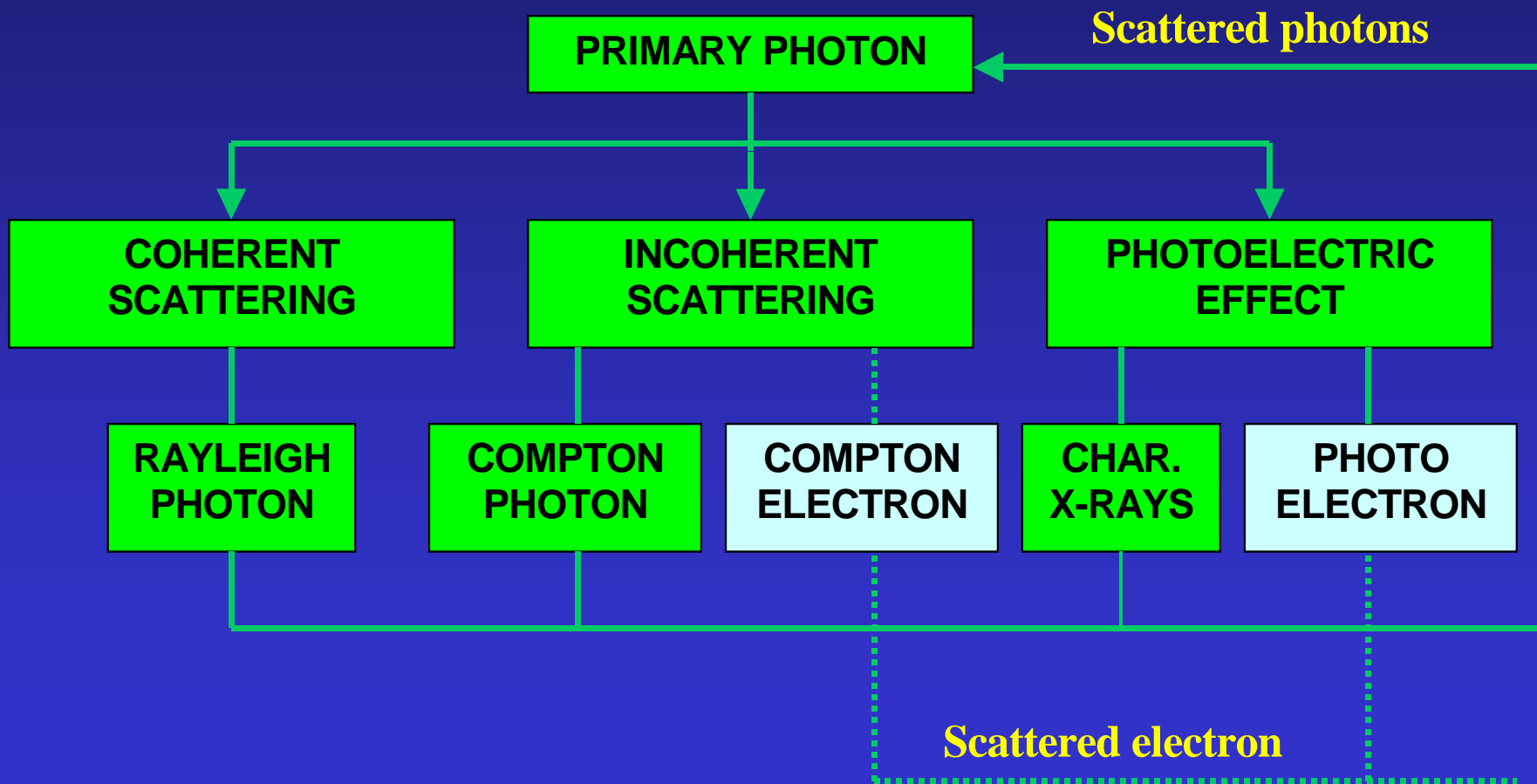
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Spectrum build-up (code SHAPE)

- **The first three collisions** give the major contribution to the x-ray spectrum
- The detector can be simulated with a **detailed response** function including **escape peaks** and non uniform efficiency
- Polarization state of the source can be: **unpolarized/linearly polarized**
- The spectrum can be digitized to **simulate acquisition with a multichannel analyzer** as in EDXRF

PREVAILING INTERACTIONS IN THE X-RAY REGIME



Using SHAPE (declaring set-up)

The screenshot shows the SHAPE software interface with the following sections and parameters:

- Shape**: Geometry, Source, Detector&MCA, Polariz.
- Set-Up**: A menu with options: Define, Retrieve, Save.
- Options**: Report, Target.
- Quit**: SHAPE v 2.18, Copyright 1989-2002, For more information see the Info issue under Options.

Section	Parameter	Value
Geometry	θ_0	45.00
	ϕ_0	0.00
	$180-\theta$	45.00
	ϕ	0.00
Source	E_0	60.00
	d_1	0.00
Detector&MCA	d_2	0.00
	Crystal	GE
	Escape Peak	<I>
	Channels	1024
	ZERO	0.00
	GAIN	0.1000
	LDis	0.00
UDis	1023.00	
Polariz.	Polariz.	<I>
	St.	<UNPOL.>

Report options:

Order	FILE
1st-order	<I>
2nd-order	<I>
3rd-order	<I>
4rd-order	<I>
Total	<I>

Target options:

H	1	0.1109
0	8	0.8800
H0	67	0.0091
..
..
..
..
..

geometry

source energy

detector & MCA

target

source polarization state

current set-up window

Using SHAPE (declaring target)

The screenshot shows the SHAPE software interface with the following sections:

- Shape**: Geometry (θ₀ = 45.00, φ₀ = 0.00, 180-θ = 45.00, φ = 0.00), Source (E₀ = 60.00, d₁ = 0.00), Detector&MCA (d₂ = 0.00, Crystal = GE, Escape Peak <I>, Channels = 1024, ZERO = 0.00, GAIN = 0.1000, LDis = 0.00, UDis = 1023.00).
- Set-Up**: **Define** (selected), Report, File.
- Options**: (Empty)
- Quit**: (Empty)

The **Define** menu is open, showing the **Composition** table:

1.	H	1	0.1109
2.	O	8	0.8800
3.	H ₂ O	67	0.0091
4.		0	0.0000
5.		0	0.0000
6.		0	0.0000
7.		0	0.0000
8.		0	0.0000
9.		0	0.0000
10.		0	0.0000
Total			=0.0000
Rest			=1.0000

Below the composition table, the text reads: "Choose target composition. [F2] for a table of elements".

On the right side of the interface, the following text is displayed:

SHAPE v 2.18
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Not for commercial use
For more information see the Info issue under Options

Using SHAPE (declaring geometry)

The screenshot shows the SHAPE software interface. The window title is "SHAPE - SHAPE". The menu bar includes "Shape", "Set-Up", "Options", and "Quit". The "Set-Up" menu is open, showing "Define", "Target", and "Geometry". A dialog box titled "Incidence direction" is displayed, with "Polar angle θ_0" set to 45.000 and "Azimuthal angle $\varphi_0 \equiv \theta$" set to 0.000. The main window displays various parameters and options.

Parameter	Value
θ_0	45.00
φ_0	0.00
$180 - \theta$	45.00
φ	0.00

Parameter	Value
E_0	60.00
d_1	0.00

Parameter	Value
d_2	0.00
Crystal	GE
Escape Peak	<I>
Channels	1024
ZERO	0.00
GAIN	<ESC> resets the initial value
LDis	θ_0 [deg] [0.00.. 89.99] 45.000
UDis	

Order	Material	Thickness	Order	Material	Thickness
0	8	0.8800			
H0	67	0.0091			
..			
..			
..			
..			

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Polar angle measured about the normal to the outer surface [DEGREES]

Using SHAPE (declaring source)

The screenshot shows the SHAPE software interface with the following sections:

- Shape**:
 - Geometry: $\theta_0 = 45.00$, $\varphi_0 = 0.00$, $180-\theta = 45.00$, $\varphi = 0.00$
 - Source: $E_0 = 59.54$, $d_1 = 0.00$
 - Detector&MCA: $d_2 = 0.00$, Crystal GE, Escape Peak <I>, Channels 1024, ZERO = 0.00, GAIN = 0.1000, LDis = 0.00, UDis = 1023.00
- Set-Up**:
 - M: $\langle P \rangle$, $\langle P \rangle$, $\langle P \rangle$, $\langle R \rangle$, $\langle C \rangle$, $\langle R, R \rangle$, $\langle C, C \rangle$, $\langle R, C \rangle$, $\langle C, R \rangle$, $\langle P, P, P \rangle$, $\langle P, P, P, P \rangle$
 - Energy State: U <>, LP <I>
 - Polariz.: Polariz. <I>, St. <LP= 0>
- Options**:
 - Report: FILE, order <I>, order <I>, order <I>, order <>, al <I>
 - Target: 1 0.1109, 8 0.8800, 67 0.0091, .., .., ..
- Quit**: SHAPE v 2.18, (c) JEF 1989-2002, All rights reserved, Not for commercial use, For more information see the Info issue under Options

A callout box with an arrow points to the 'LP <I>' option in the 'Polariz.' section, with the text: "changed source polarization state".

Linearly polarized (i.e. 90 degrees s beam)

Using SHAPE (switching interactions on/off)

The screenshot shows the SHAPE software interface with the following sections:

- Shape**: Geometry parameters (θ₀, φ₀, 180°, σ, E₀, d₁) and Detector&MCA parameters (d₂, Crystal, Escape Peak, Channels, ZERO, GAIN, LDis, UDis).
- Set-Up**: MS Terms and Polariz. St. (LP= 0).
- Options**: Report (Device, FIL, 1st-order, 2nd-order, 3rd-order, 4rd-order, Total) and Target (H, O, H₀).
- Interactions**: A list of interaction types with checkboxes. The '(P,C)' option is highlighted in pink.
- Quit**: A section containing text: 'reserved for commercial use' and 'information see under Op-'. The text 'PHOTOELECTRIC photons COMPTON scattered towards the detector (continuous)' is also visible at the bottom.

A white arrow points to the '(P,C)' option in the Interactions list with the text "changed interaction".

Interaction	Checked
(P)	<input type="checkbox"/>
(R)	<input type="checkbox"/>
(C)	<input type="checkbox"/>
(P,P)	<input type="checkbox"/>
(P,R)	<input type="checkbox"/>
(P,C)	<input checked="" type="checkbox"/>
(R,P)	<input type="checkbox"/>
(C,P)	<input type="checkbox"/>
(R,R)	<input type="checkbox"/>
(C,C)	<input type="checkbox"/>
(R,C)	<input type="checkbox"/>
(C,R)	<input type="checkbox"/>
(P,P,P)	<input type="checkbox"/>
(P,P,P,P)	<input type="checkbox"/>

Using SHAPE (computing)

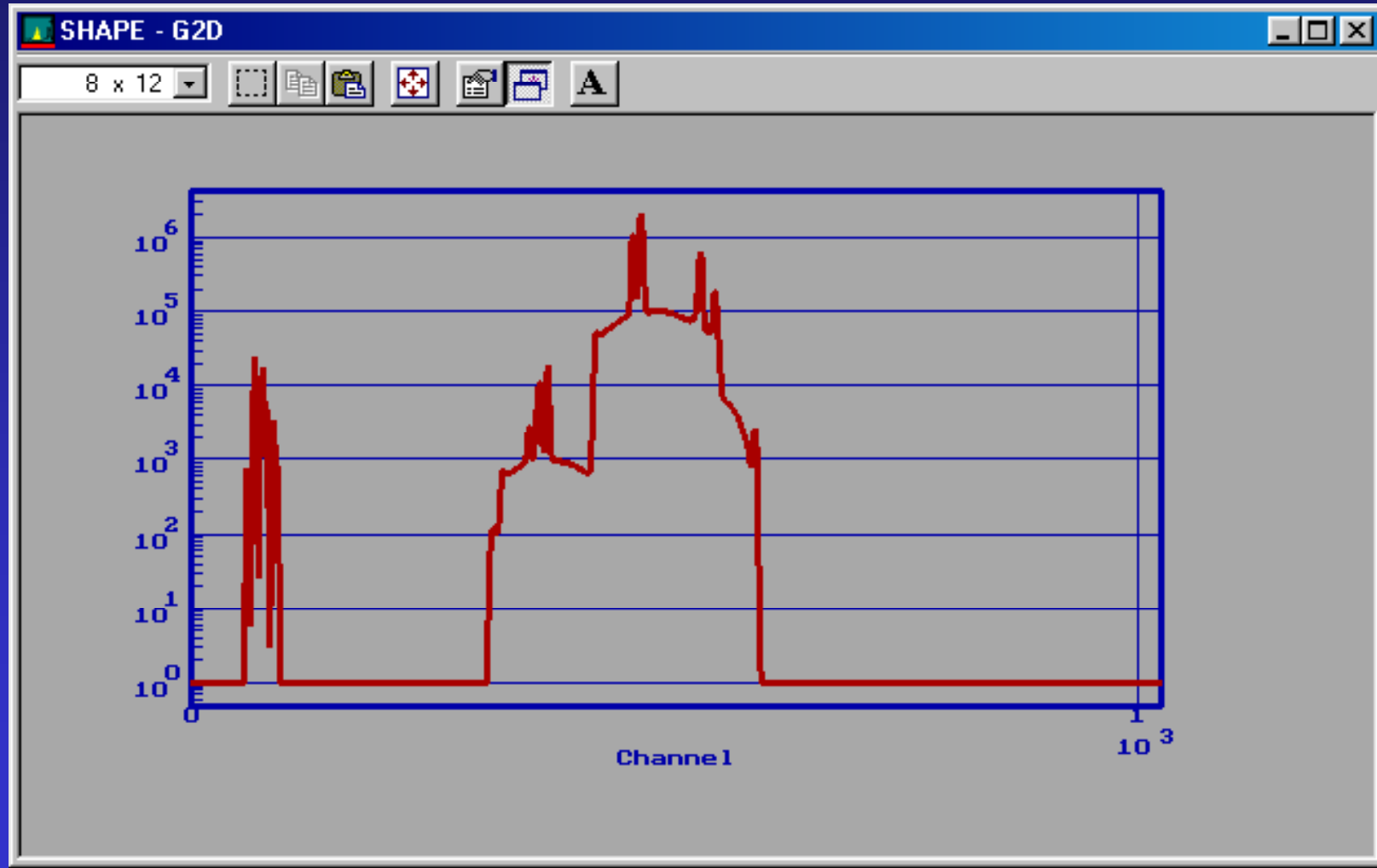
The screenshot shows the SHAPE software interface. The title bar reads "SHAPE - SHAPE". The menu bar includes "Shape", "Set-Up", "Options", and "Quit". The "Shape" menu is open, showing options: "Compute", "Plot", "Report", and "Attenuation". The "Compute" option is highlighted. Below the menu, there are sections for "Source" and "Detector&MCA". The "Source" section shows $E_0 = 59.54$ and $d_1 = 0.00$. The "Detector&MCA" section shows $d_2 = 0.00$, "Crystal GE", "Escape Peak ()", "Chan", "ZERO", "GAIN", "LDis", and "UDis". A white text box with a black border is overlaid on the interface, containing the text "computation is completed with detector influence". The main window displays a table of MS Terms and an I/O Window. The table has columns for "MS Terms" and "I/O Window". The "I/O Window" section shows a list of lines with their corresponding energy values and widths.

MS Terms	I/O Window
(P) (I)	Line : H0 K α 1 --Total-- <f2=19.26%> < 4
(R) (I)	7.545 KeV
(C) (I)	Width [eV] = 31.10
(P,P) (I)	Line : H0 K β 3 --Total-- <f2=19.08%> < 5
(P,R) (I)	3.709 KeV
(P,C) ()	Width [eV] = 33.85
(R,P) (I)	Line : H0 K β 1 --Total-- <f2=19.07%> < 5
(C,P) (I)	3.875 KeV
(R,R) (I)	Width [eV] = 34.47
(C,C) (I)	Line : H0 K β 2 --Total-- <f2=19.03%> < 5
(R,C) (I)	5.318 KeV
(C,R) (I)	Width [eV] = 64.60
(P,P,P) (I)	Line : H0 LL --Total-- <f3= 0.01%> < 5
	5.943 KeV
	Width [eV] = 13.83
	Line : H0 L α 2 --Total-- <f3= 0.01%> < 5
	6.679 KeV

computation is completed with detector influence

Perform spectral build up according to multiple scattering theory

Using SHAPE (plotting)



using SHAPE with a polychromatic source

- 1) create the new directory TEST and move into it; then create the directory SPEC
- 2) in TEST create one *.SET file for each energy bin
- 3) create the file SPECT.BAT

```
FOR %%I IN (*.SET) DO CALL ONEBIN %%I
```

- 4) create the file ONEBIN.BAT

```
..\SHAPE %1 1  
MOVE 123D.DAT SPEC\%1  
DEL DEFAULT.SET
```

CODES COMPARISON (part 1: Physics)

Features	Details	SHAPE v2.20	D3DSHAPE v1.0	MCSHAPE v2.04	
	photoelectric effect	☒	☒	☒	
	~1000 characteristic lines	☒	☒	☒	
	line width	☒		☒	
	atomic Rayleigh scattering	☒	☒	☒	
	atomic Compton scattering	☒	☒	☒	
	Compton profile	first collision only		☒	☒
Physics	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			☒		

CODES COMPARISON (part 2: model and programming)

Features	Details	SHAPE v2.20	D3DSHAPE v1.0	MCSHAPE v2.04
Miscellaneous	selective computation of single interaction chains	☒	partial	foreseen in v3
Transport model	particle	photons	photonsselectrons	photons
	scalar equation	☒	☒	
	vector equation	☒		☒
	solution	deterministic	deterministic	Monte Carlo
	collisions	3	3	100
	1-D spatial geometry	☒		☒
	3-D spatial geometry		☒	foreseen in v3
Code	language	DELPHI	FORTRAN 77	FORTRAN 90
	additional libraries	graphics		WINTERACTER
	platform	DOSWINDOWS	LINUX	WINDOWSLINUX
	distribution	web site	alpha testing	web site
	parallelization			MPICH v1.0 (only Linux)
Applications	spectroscopy	☒	☒	☒
	analytical chemistry	☒	☒	☒
	radiation metrology	☒	☒	☒
	radiation shielding	☒	☒	☒
	dosimetry		foreseen in v2	foreseen in v3
	radiation transport teaching	☒		☒



CONCLUSIONS

X-ray photon transport is a good benchmark for transport theory because:

- **the transport equation for photons is linear (is analogous to the neutron transport equation)**
- **the interactions involved are both, isotropic (photoelectric characteristic emission) and anisotropic (Rayleigh and Compton scattering)**
- **the spectroscopic application obliges to maintain the full energy and angle distributions**