THE DETERMINISTIC CODE
SHAPE

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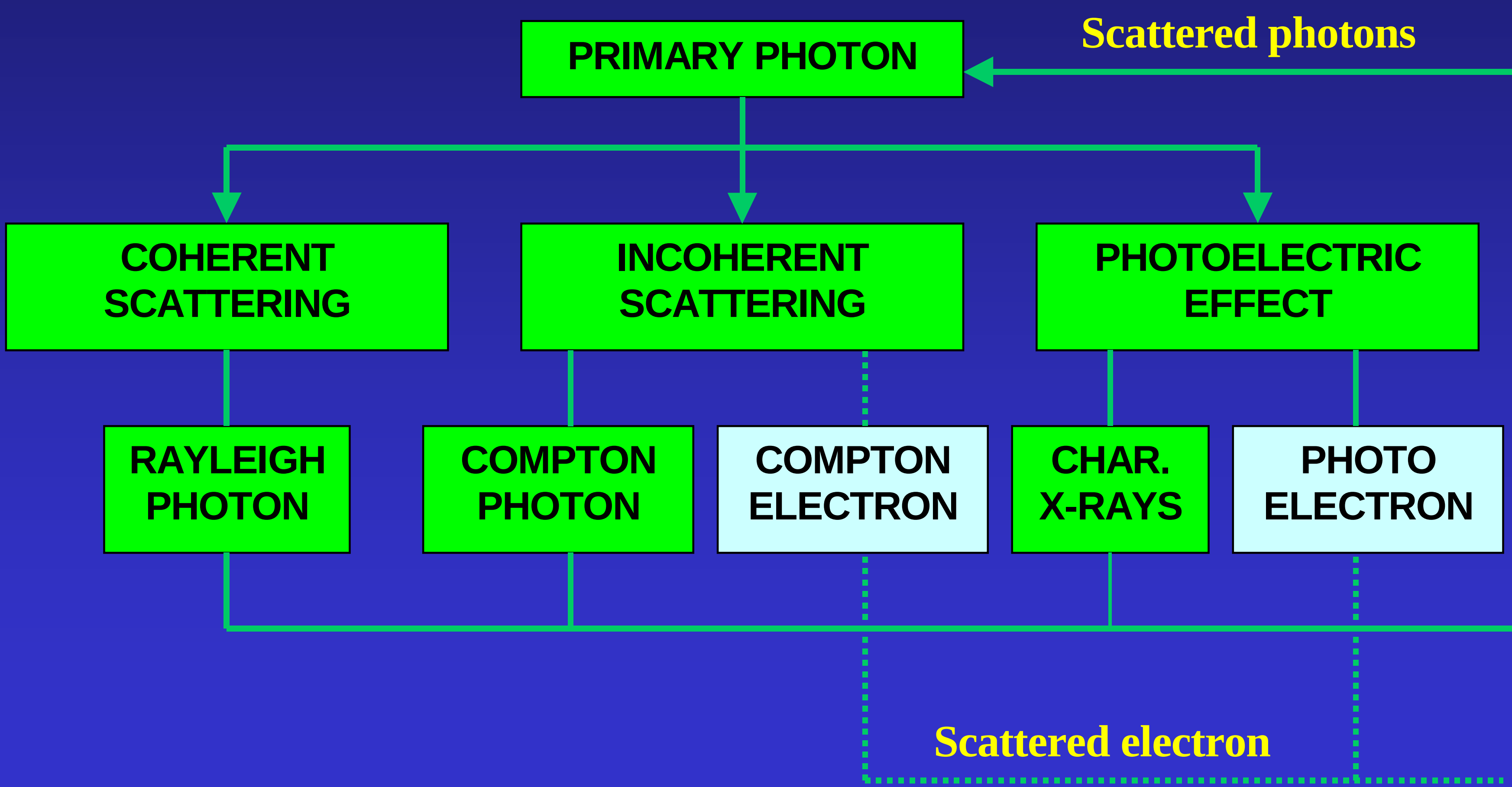
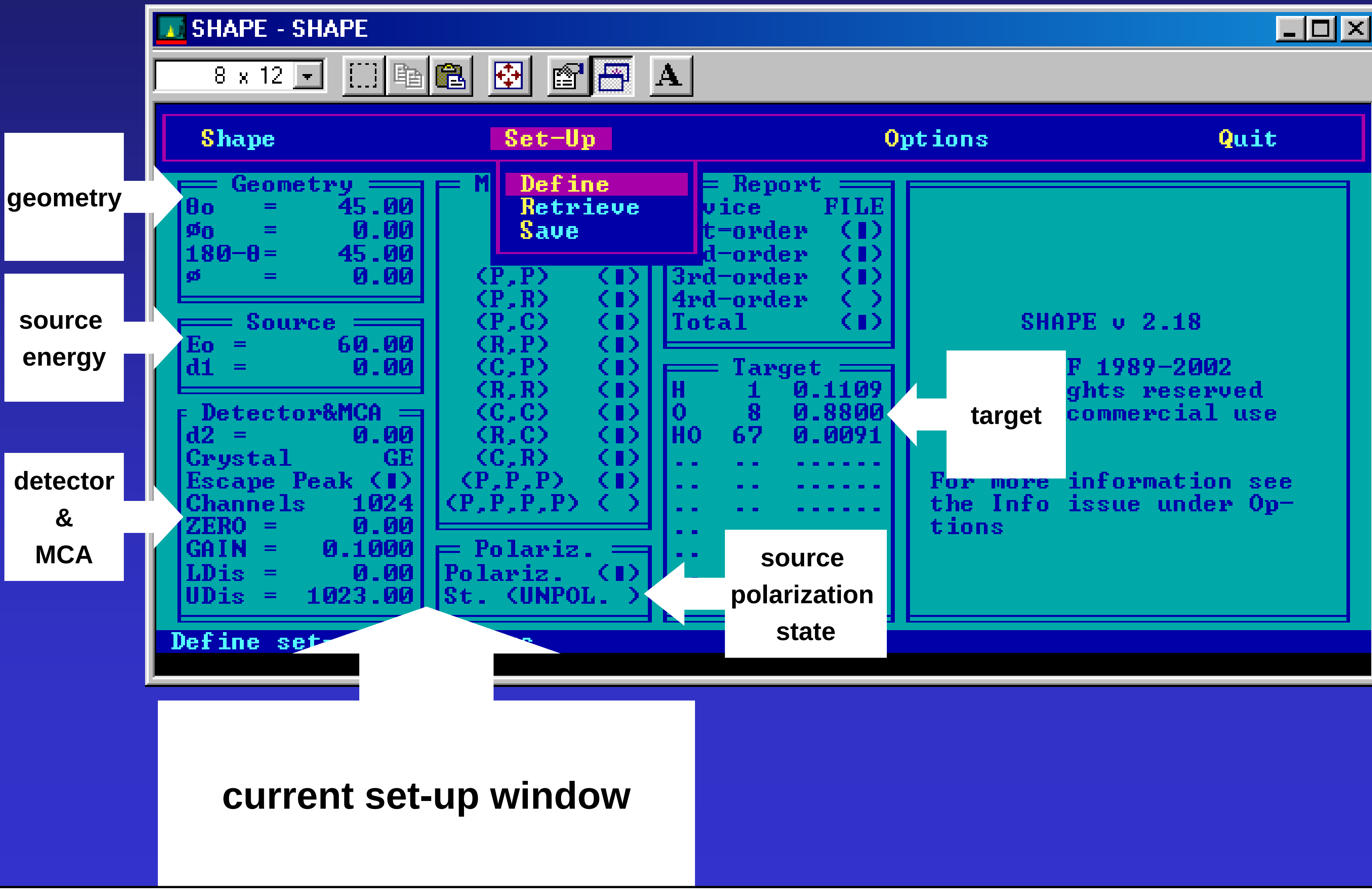
Spectrum build-up (code SHAPE)

- 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

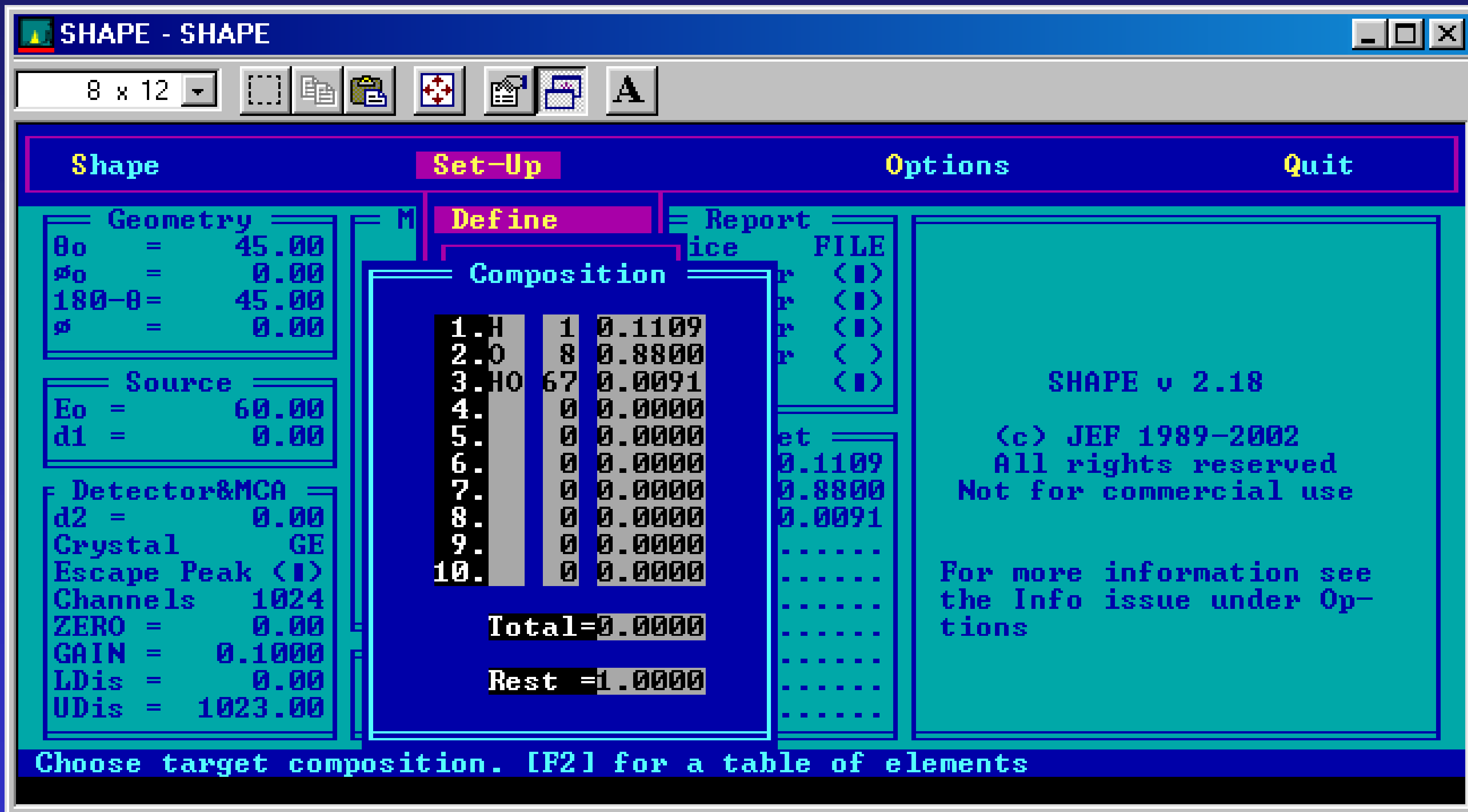
PREVAILING INTERACTIONS IN THE *X-RAY* REGIME



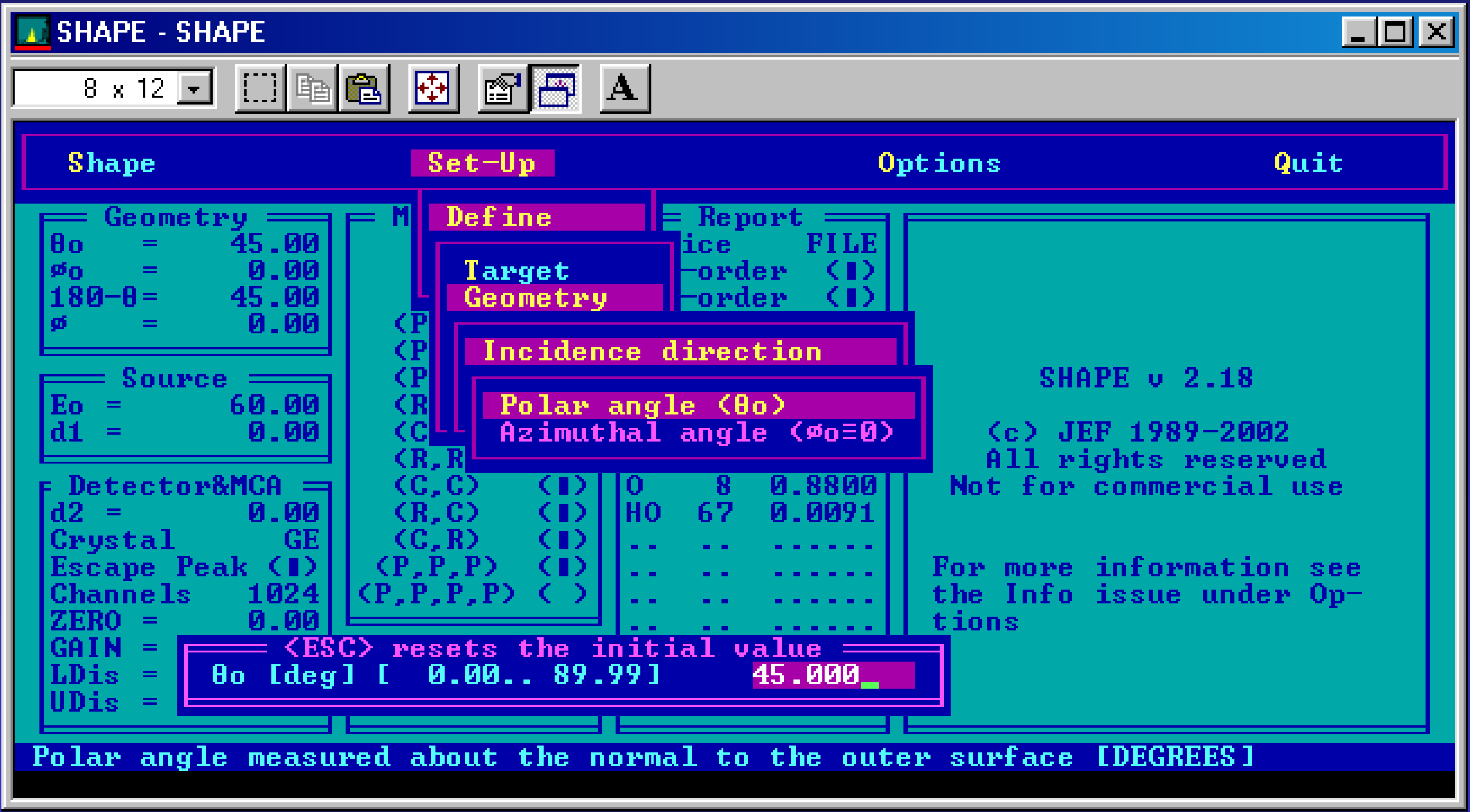
Using SHAPE (declaring set-up)



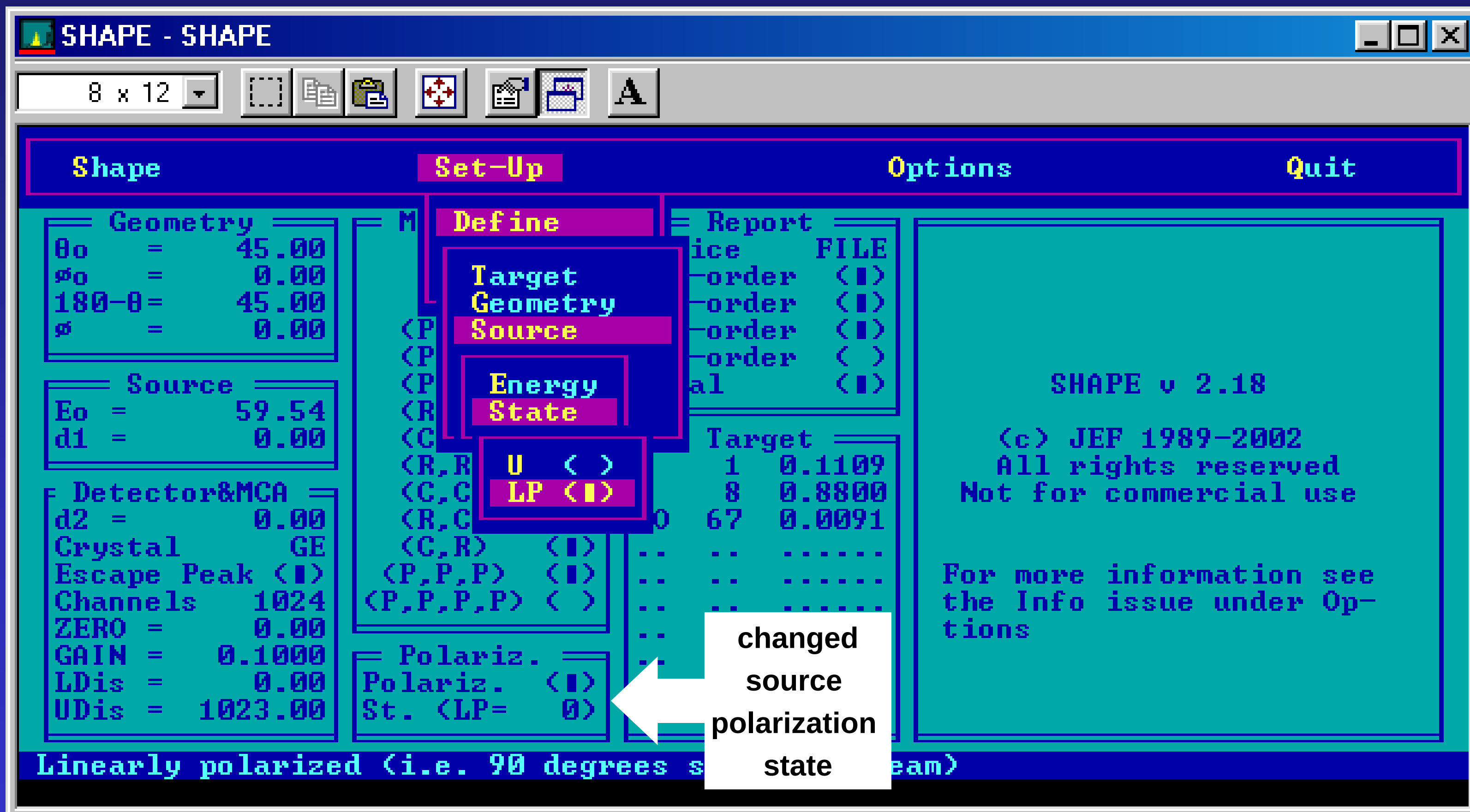
Using SHAPE (declaring target)



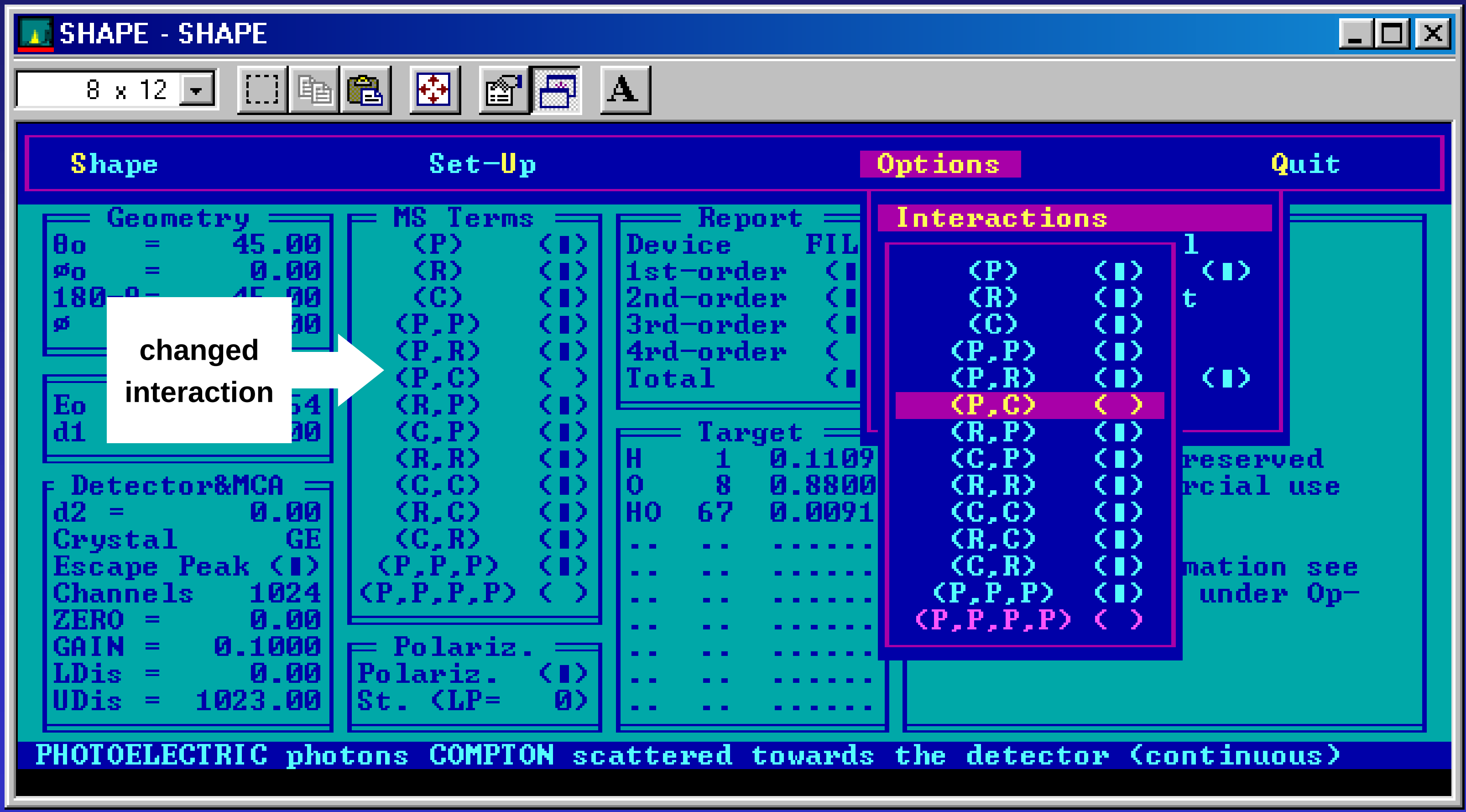
Using SHAPE (declaring geometry)



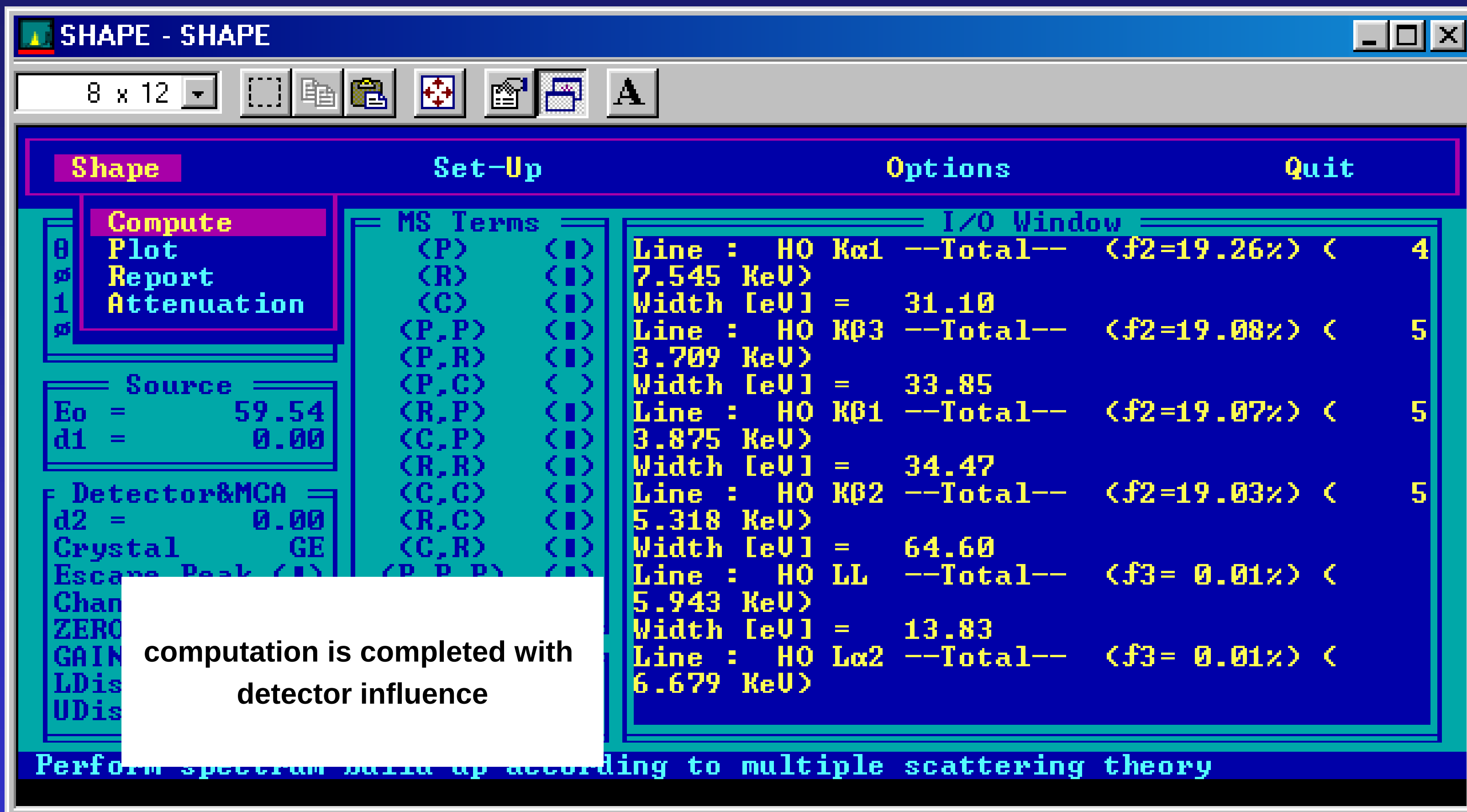
Using SHAPE (declaring source)



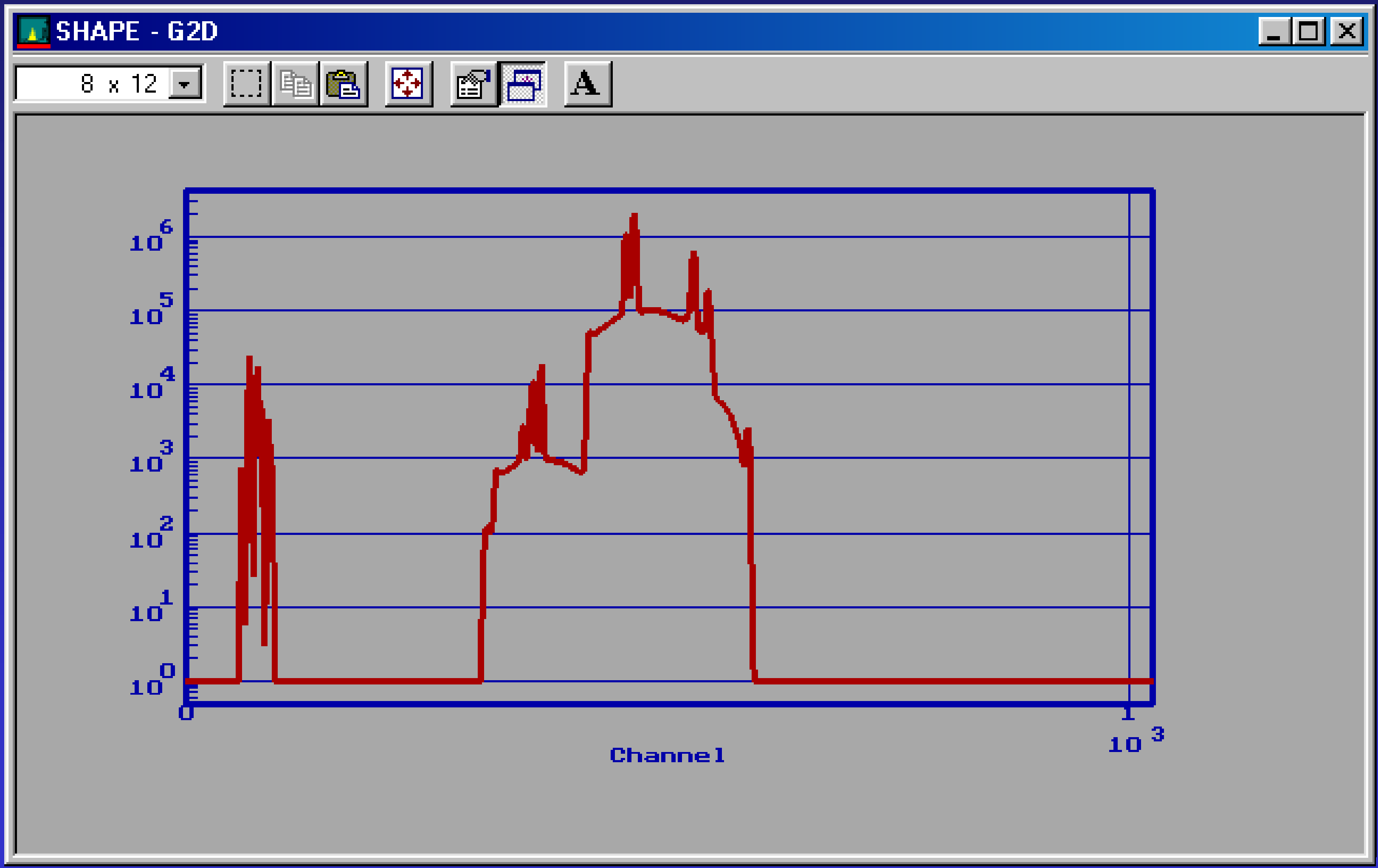
Using SHAPE (switching interactions on/off)



Using SHAPE (computing)



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
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			☒

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	photonselectrons	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