A Guide to the "X-ray Map Simulator" Tool in Lispix

The Lispix "X-ray Map Simulator" is a visibility predictor

- With quantitative elemental x-ray mapping becoming an increasingly attractive tool, we need to understand the limitations for a particular measurement situation, e.g.,

    1. How many counts per pixel are needed to recognize a compositional feature?

    2. How does feature size relative to image frame matter?

    3. For the particular element and measurement conditions, what minimum concentration level can we reliably observe in an image?

- Predicting visibility has two parts:

    1. We need to have appropriate x-ray counts for the compositional object and the background material. While experimental values can be used, in general such values will not be available, so we must simulate the spectrum. An EDS spectrum simulator such as NIST DTSA (Fiori, Myklebust, and Swyt) for the Macintosh platform or Nicholas Ritchie's "Son of DTSA" for the pc platform can be used.

For DTSA:

    – http://www.nist.gov/lispix/doc/other-software/dtsa.htm

NIST Desktop Spectrum Analyzer: Spectrum Simulator

Z	Weight Fraction	
Mg	0.08850	
Si	0.25380	
Ca	0.11060	
Fe	0.11210	
8	0.42360	
0	0	
0	0	
0	0	
0	0	
0	0	
0	0	
0	0	
0	0	

- ● Wt. Fr.
- ○ At. Fr.
- ○ # Atoms
- ○ mMol/kg
- ○ Ox. Wt. Fr.
- ○ Valences

Output Choices

Physics Choices

● EDS   ○ WDS

Detector Parameters

Channel Specs

Load Info from WORK   **Clear Output Options**

Beam kV:	20.000
NanoAmps Faraday:	0.500
Seconds, Live:	1.000
Density, g/cc:	N/A
Thickness, nm:	N/A

Load a Database   **Make a DataBase**   **Insert item**   **Remove item**

Enter Here name of new item in database (<32 chars)

```
1  K227
2  K309
3  K411
4  K412
5  K961
6  Quartz
7  K2063a
```

Zero All

Av Z= 13.13060   Sum= 0.98860   1-Sum= 0.01140

Help   **Cancel**   **Generate**

The Basis for the Generated X-ray intensity

$$I_{gen} = (\omega\, N_A\, \rho\, C_i\, /A)\, R \int_{E_c}^{E_0} (Q\, /\, (dE/ds)\, dE$$

ω = fluorescence yield N_A = Avogadro's number

ρ = density C_i = mass concentration of i

A = atomic weight   R = backscatter loss

Q = ionization cross section

dE/ds = rate of energy loss
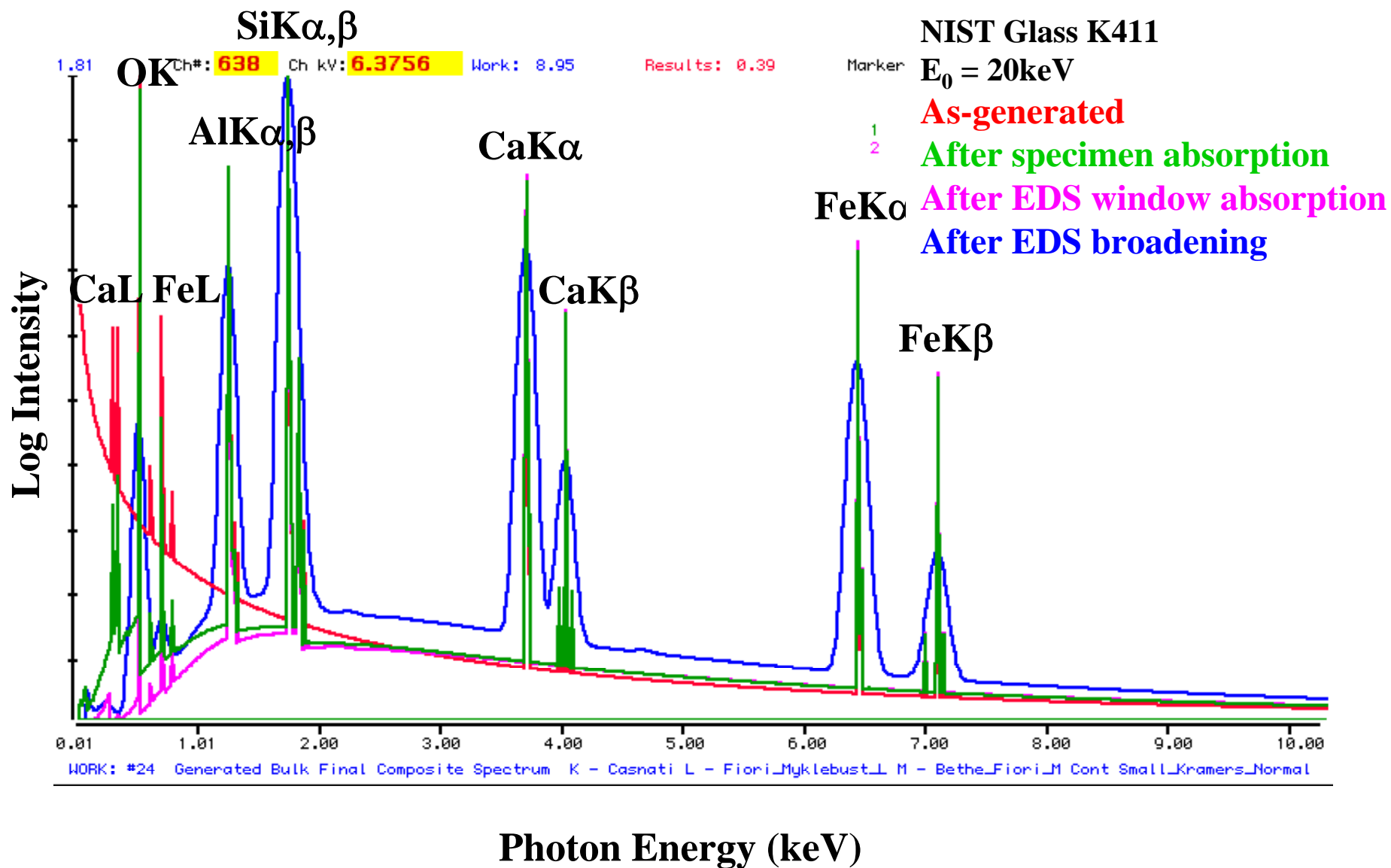
E_0 = incident beam energy E_c = excitation energy

At each photon energy, calculate the specimen absorption:

$$I_{measured} = I_{generated} * f(\chi) * \varepsilon$$

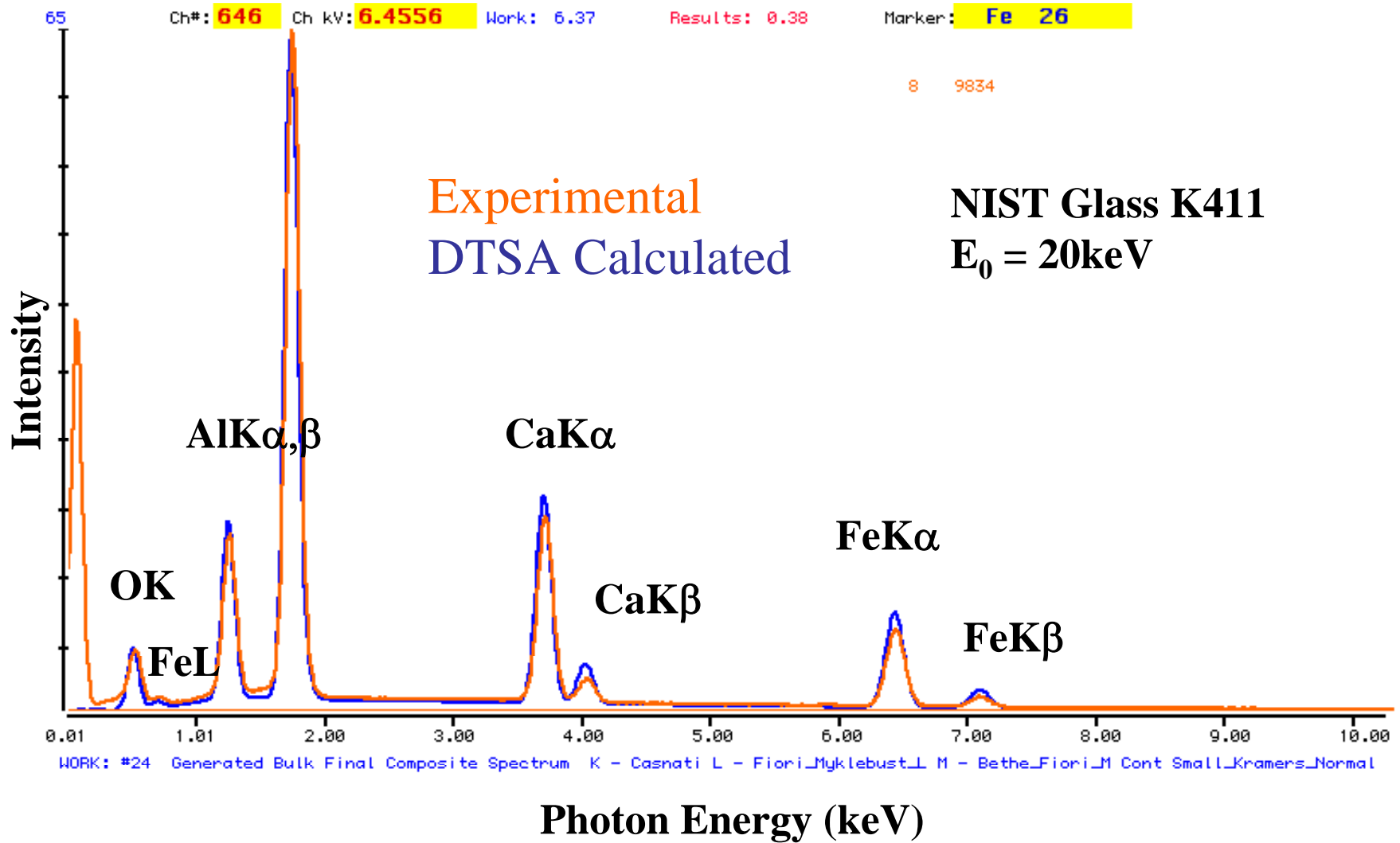$f(\chi)$ = absorption over depth distribution, x-ray fraction emitted

ε = detector efficiency

DTSA Spectrum Simulator:
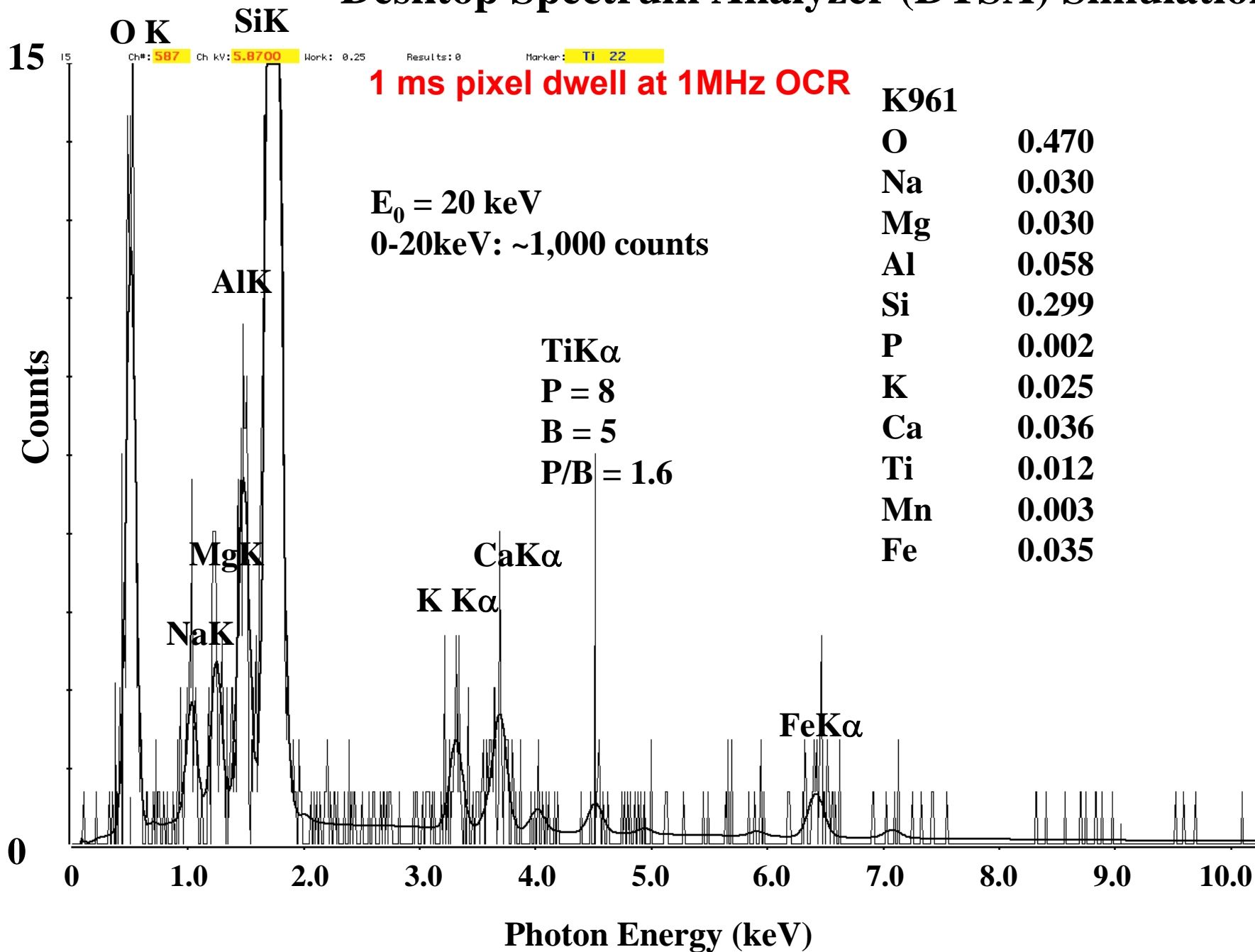## Spectra of NIST SRM Glass K411 at Various Stages

NIST Glass K411
$E_0 = 20keV$
As-generated
After specimen absorption
After EDS window absorption
After EDS broadening

SiKα,β

OK

AlKα,β

CaKα

FeKα

CaKβ

CaL FeL

FeKβ

1.81 Ch#: **638**   Ch kV: **6.3756**   Work: 8.95   Results: 0.39   Marker

Log Intensity

0.01   1.01   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00   10.00

WORK: #24   Generated Bulk Final Composite Spectrum   K - Casnati L - Fiori_Myklebust M - Bethe_Fiori_M Cont Small_Kramers_Normal

Photon Energy (keV)

DTSA Spectrum Simulator:
Measured and Simulated Spectra of NIST SRM Glass K411

SiKα,β

Ch#: **646**   Ch kV: **6.4556**   Work: 6.37   Results: 0.38   Marker: **Fe 26**

8   9834

Experimental
DTSA Calculated

NIST Glass K411
E$_0$ = 20keV

Intensity

AlKα,β

CaKα

FeKα

OK

FeL

CaKβ

FeKβ

65

0.01   1.01   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00   10.00

WORK: #24   Generated Bulk Final Composite Spectrum   K – Casnati L – Fiori_Myklebust_L M – Bethe_Fiori_M Cont Small_Kramers_Normal

Photon Energy (keV)

Desktop Spectrum Analyzer (DTSA) Simulation

1 ms pixel dwell at 1MHz OCR

O K
SiK
AlK
MgK
NaK
K Kα
CaKα
FeKα

Ch#: 587   Ch kV: 5.8700   Work: 0.25   Results: 0   Marker: Ti 22

$E_0 = 20$ keV
0-20keV: ~1,000 counts

TiKα
P = 8
B = 5
P/B = 1.6

K961	
O	0.470
Na	0.030
Mg	0.030
Al	0.058
Si	0.299
P	0.002
K	0.025
Ca	0.036
Ti	0.012
Mn	0.003
Fe	0.035

Counts

Photon Energy (keV)

- Predicting visibility has two parts:
    1. EDS spectrum predictor is needed, e.g., NIST DTSA. This estimates peak and background counts for putative objects.
    2. The x-ray image visibility predictor is based upon previous SEM image visibility research tools developed by David Bright (ref). With the counts predicted with DTSA for the characteristic peaks and continuum backgrounds, the Lispix image simulation tool constructs an image of objects with various shapes and sizes on a uniform background to create a template. Then apply Gaussian statistics appropriate to the count at each pixel to simulate image noise.

        (reference: Bright, D. S., Newbury, D. E., and Steel, E. B., "Visibility of objects in computer simulations of noisy micrographs", J. Micros., 189 (1998) 25-42.)

Step-by-step: (1) From "tools" menu, select "Xray Map Simulator"
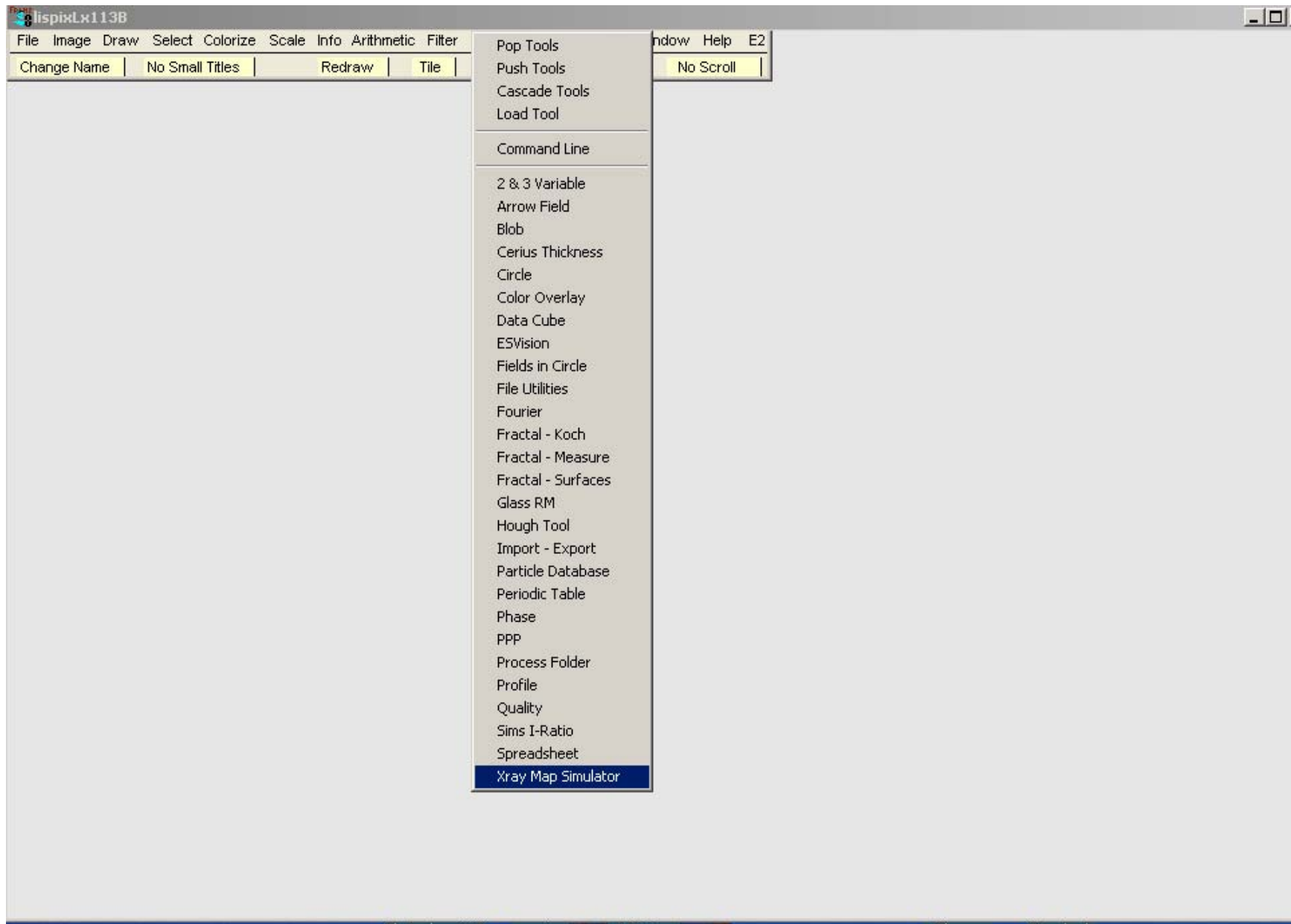
Step-by-step: (2) To create a new image, under "File" select "New list"
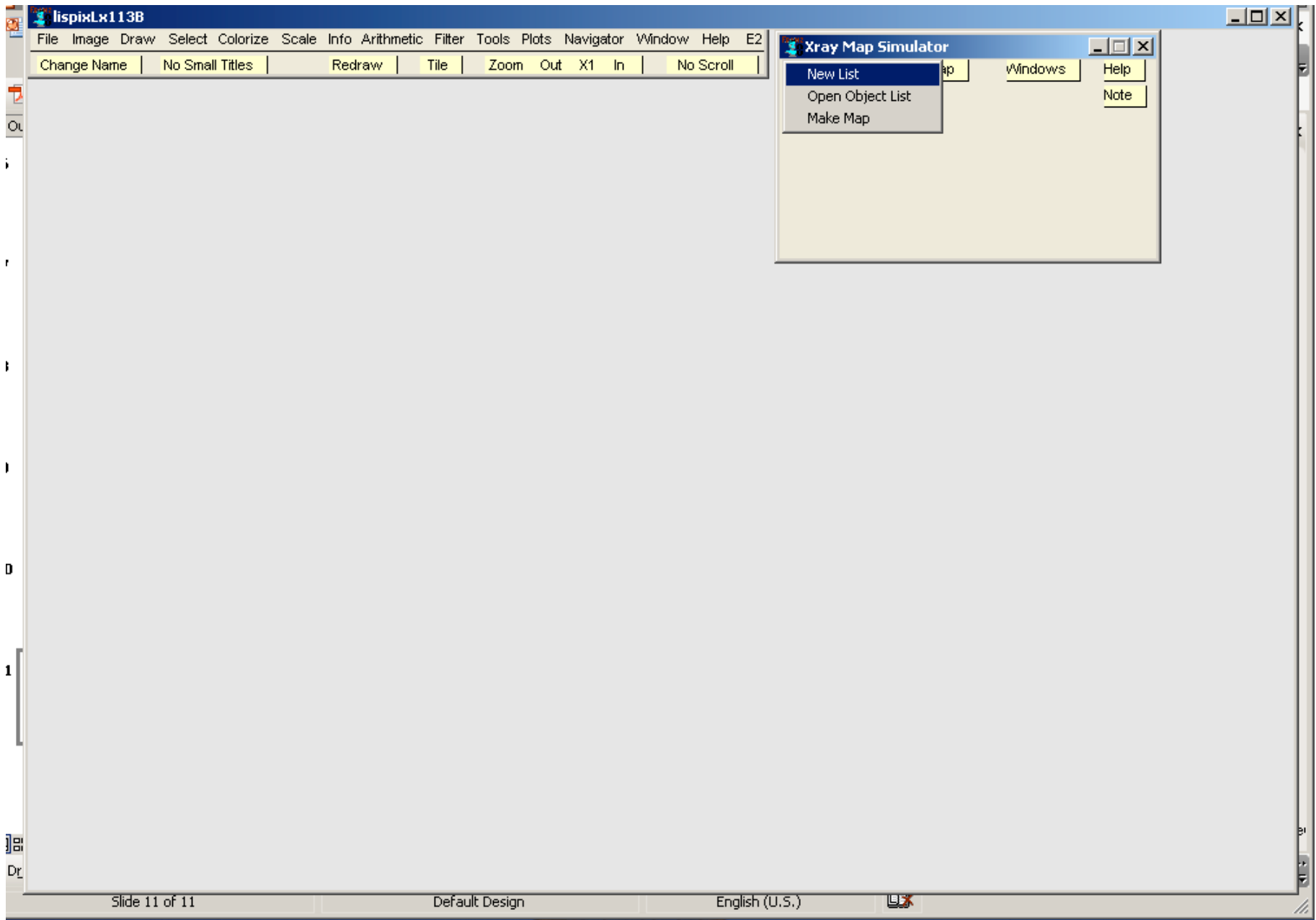
Step-by-step: (3) A series of menus will appear; note that this series of menus will create a text file "New Object List" that can be saved under the main "File" menu with the "Save Text" command.
First task: give a specific name to the "New Object List" text file of instructions.
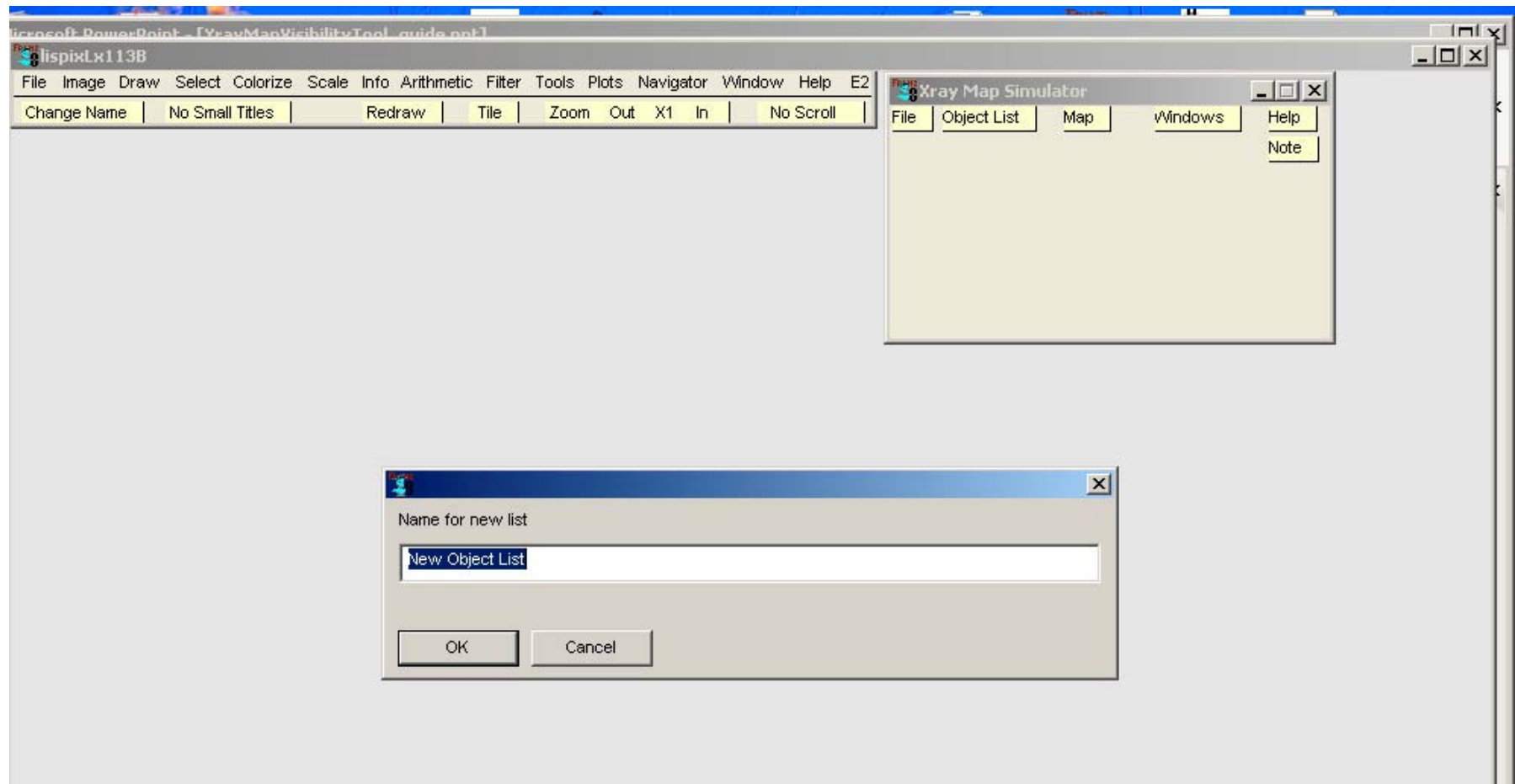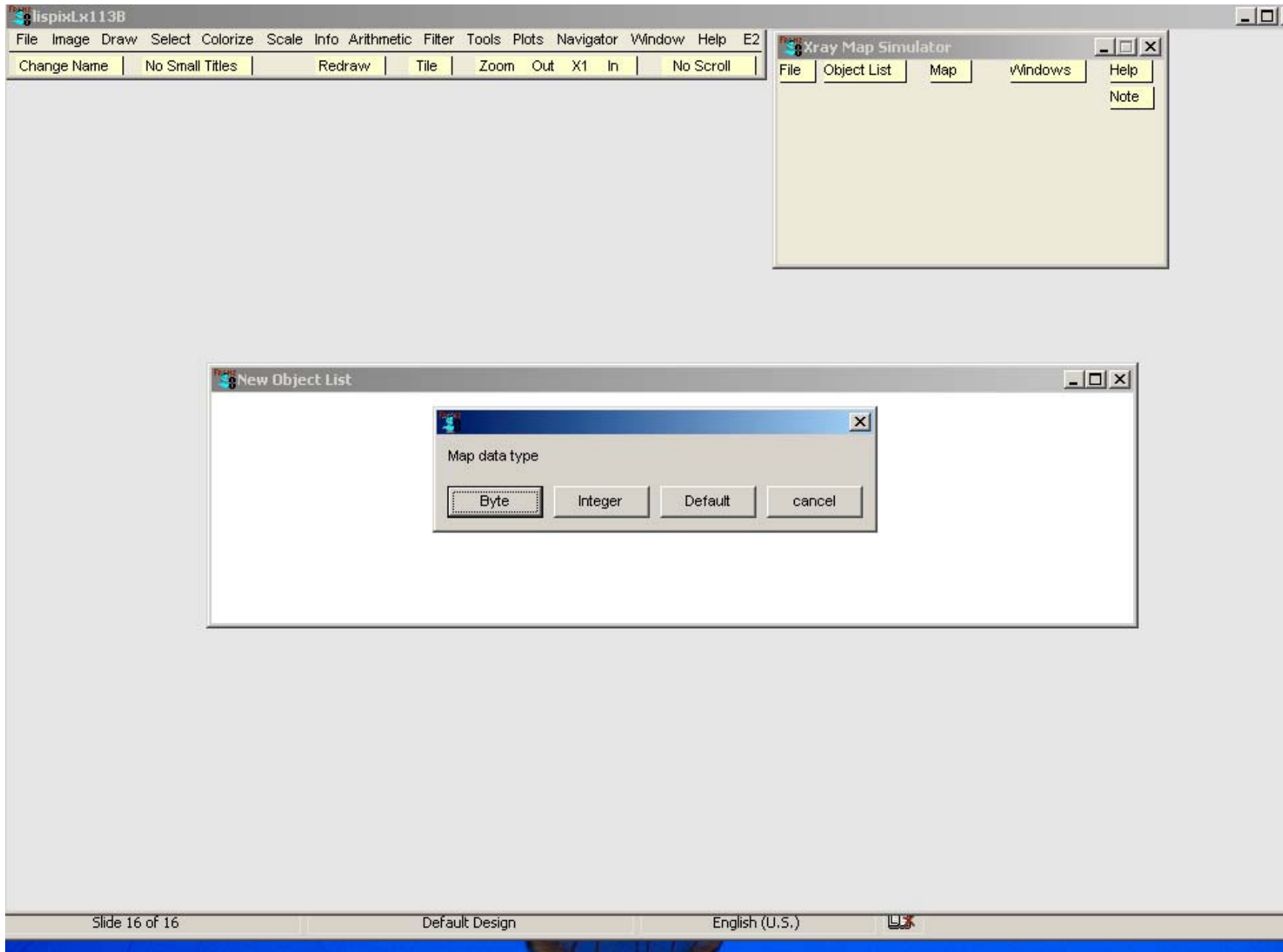
Step-by-step: (4) Choose image dimensions (default 300 x 200)
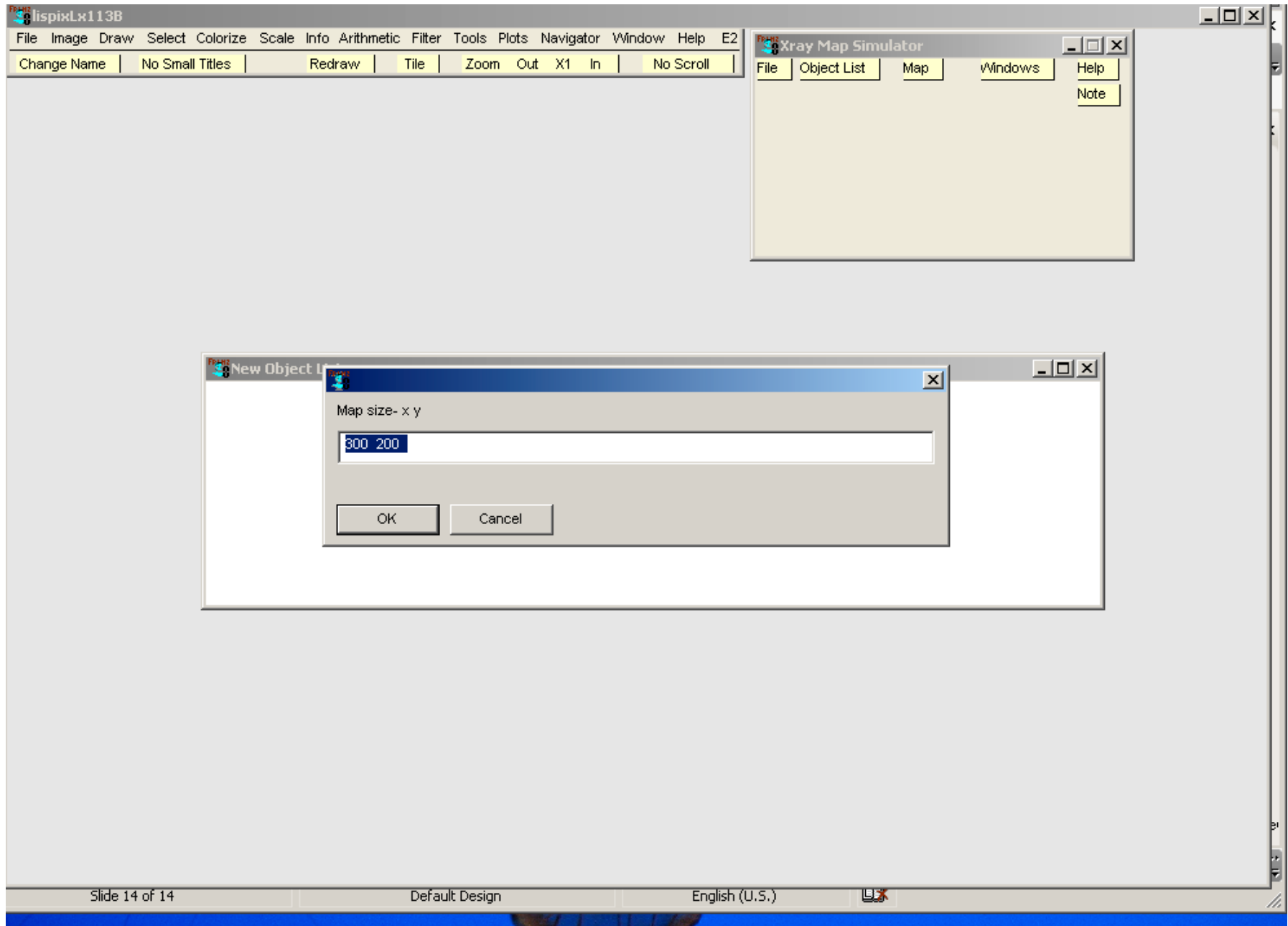
Step-by-step: (5) Choose background counts (default 15)
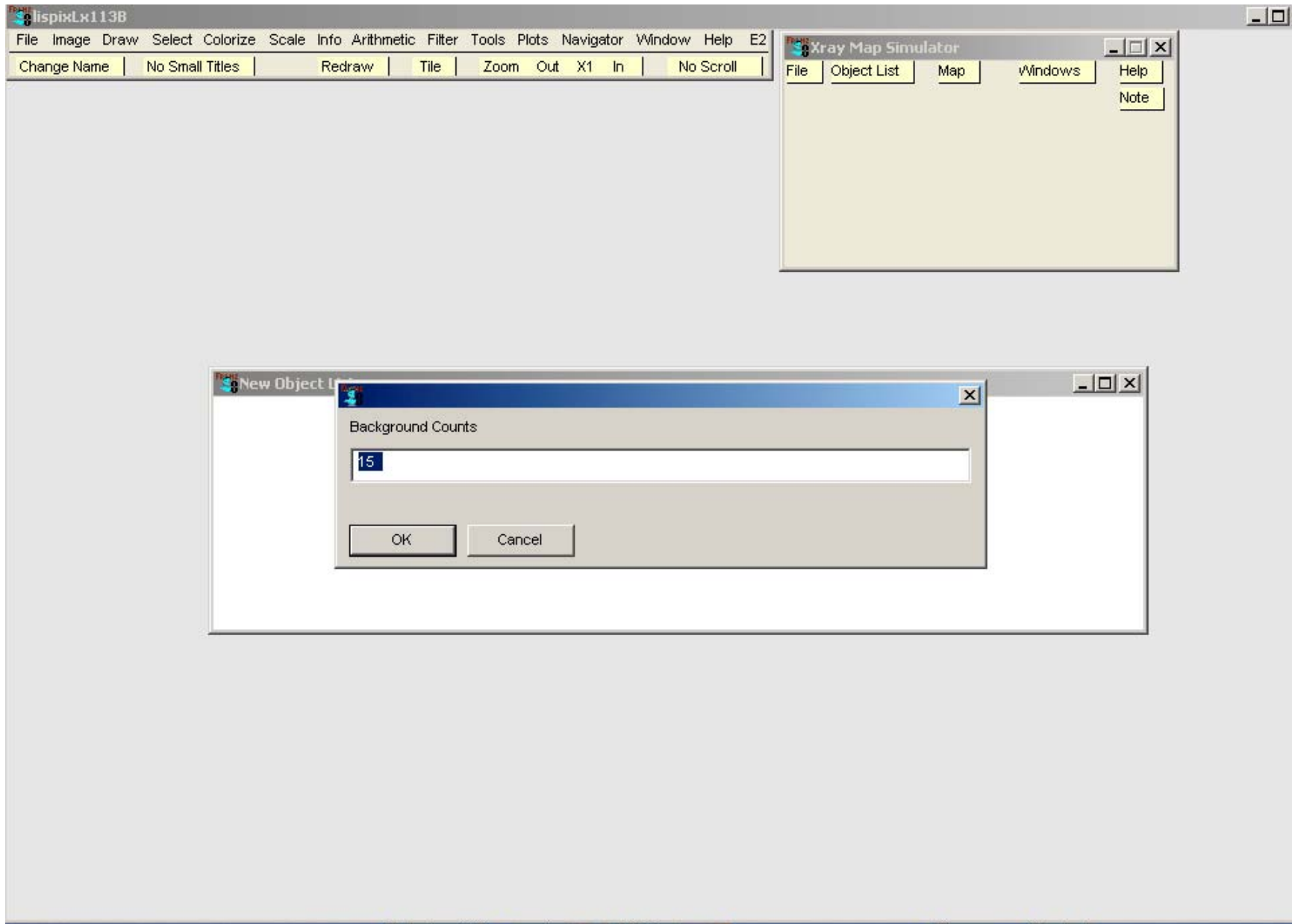
Step-by-step: (6) Choose data type

Step-by-step: (7) Choose treatment of overlapping objects, addition or replacement. This will matter for overlapping objects if the intensity of a pixel in the overlap pixels really is a sum of the intensity from objects "A" and "B", or alternatively the overlap pixel is defined entirely by the intensity of the overlaid object.
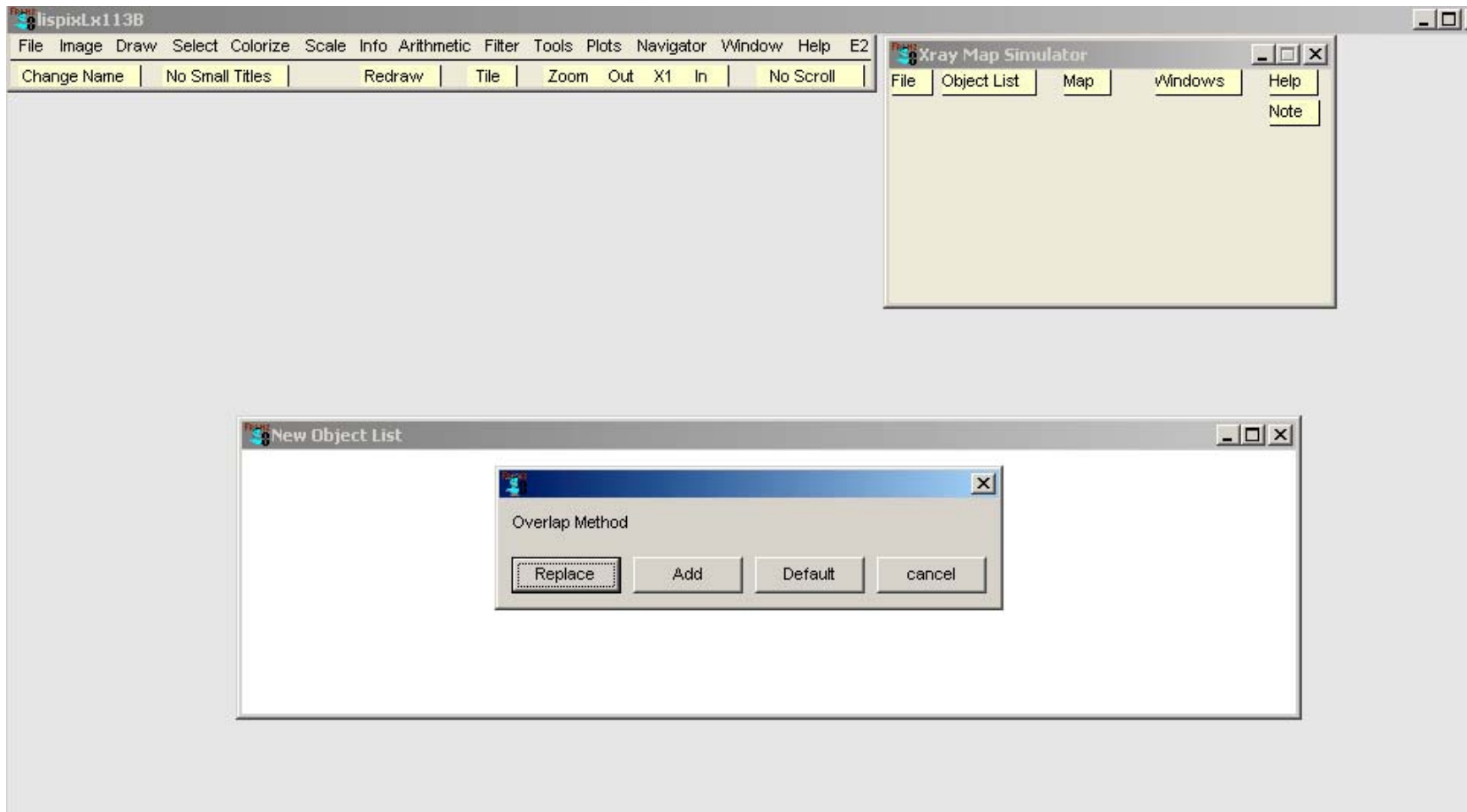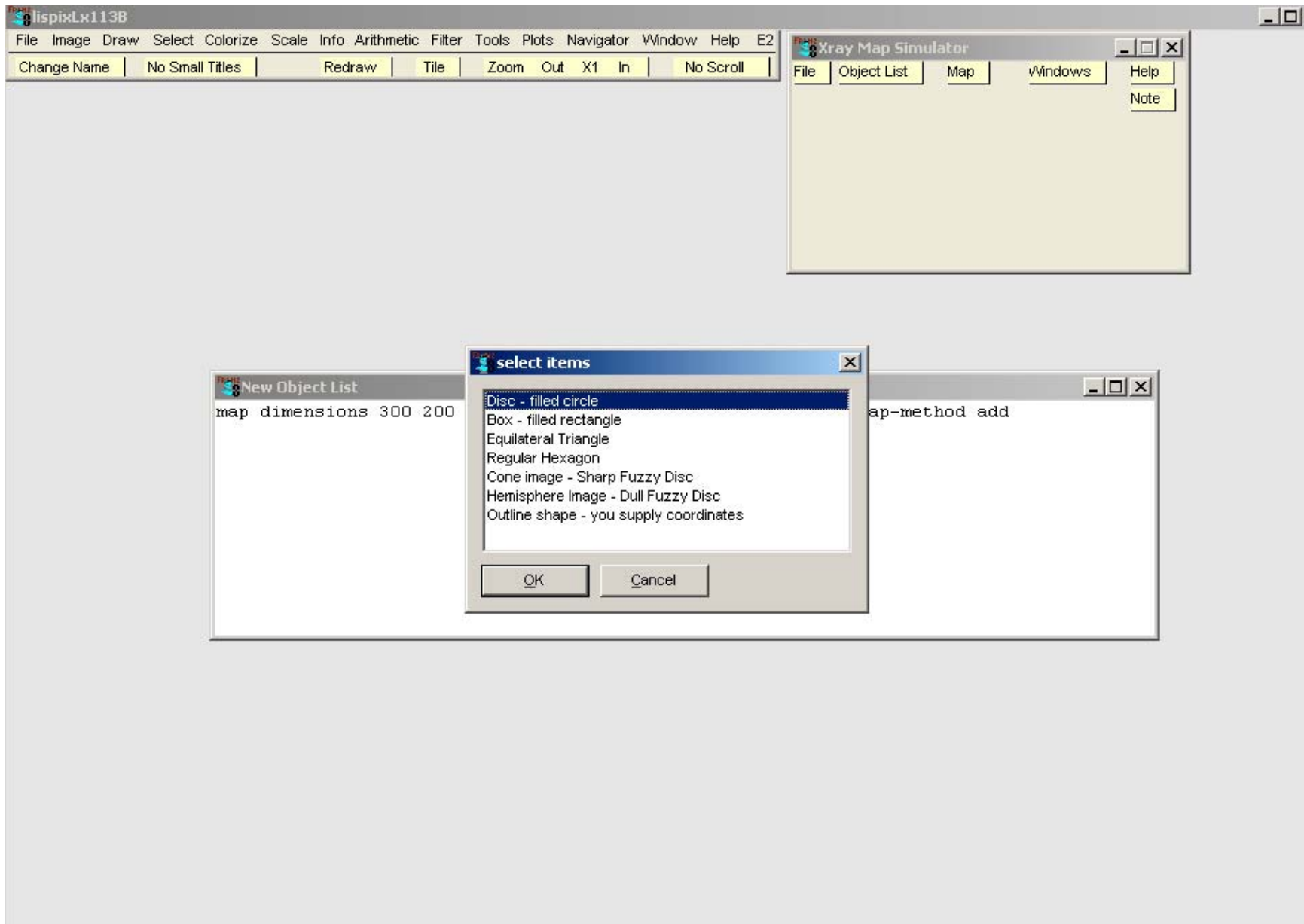
**Step-by-step: First line of file is now complete; now populate list with objects**

lispixLx113B

File Image Draw Select Colorize Scale Info Arithmetic Filter Tools Plots Navigator Window Help E2

Change Name | No Small Titles | Redraw | Tile | Zoom Out X1 In | No Scroll |

Xray Map Simulator

File | Object List | Map | Windows | Help

Note

New Object List

map dimensions 300 200   background 15   data-type byte   overlap-method add
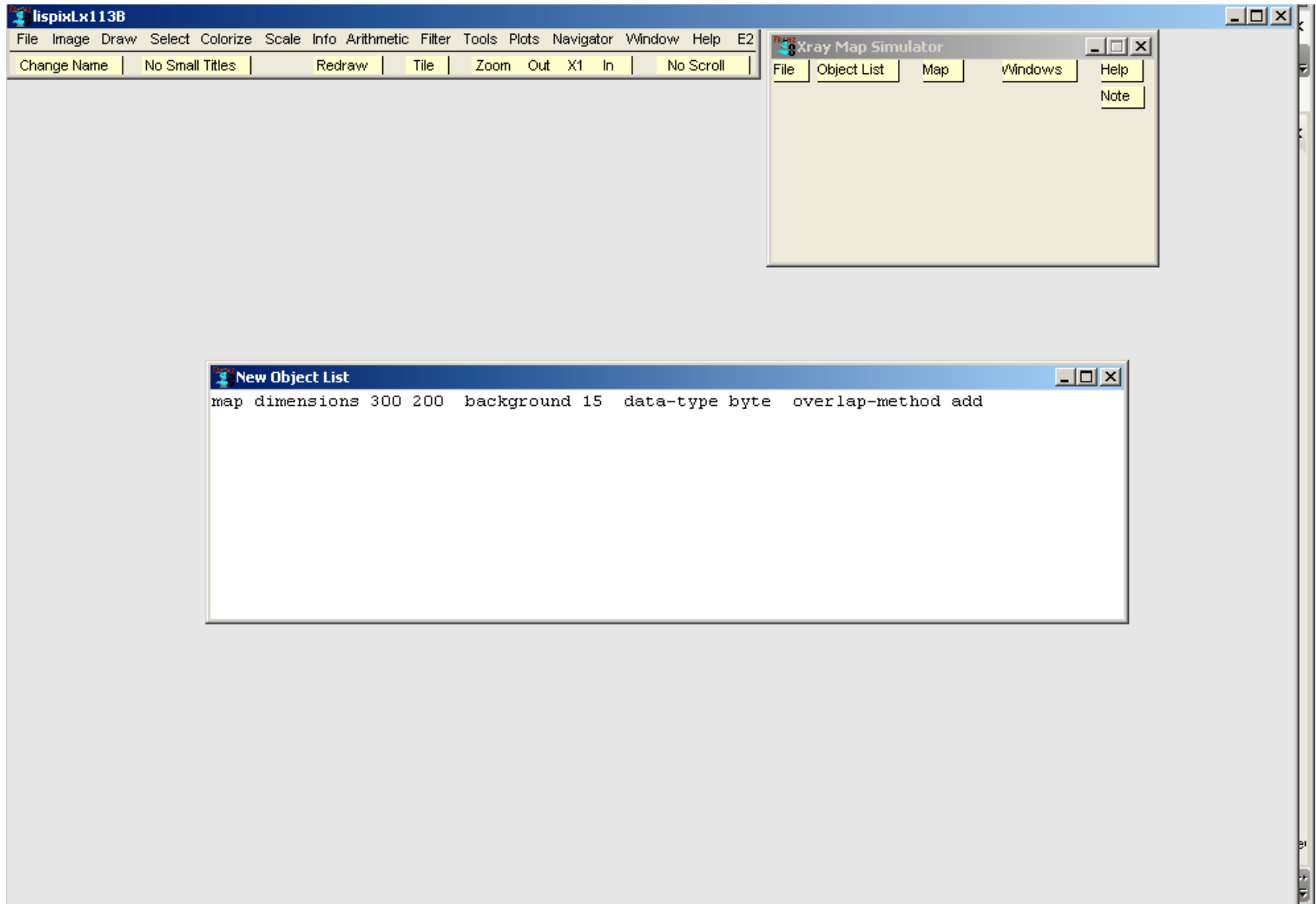
Step-by-step: (8) From "Object List" tab select "Add Sample Object – plain values"

Step-by-step: A list of choices for object shape will appear

lispixLx113B

File Image Draw Select Colorize Scale Info Arithmetic Filter Tools Plots Navigator Window Help E2

| Change Name | No Small Titles | | Redraw | Tile | Zoom Out X1 In | No Scroll |

Xray Map Simulator

| File | Object List | Map | Windows | Help |

Note

select items

New Object List

map dimensions 300 200

ap-method add

Disc - filled circle
Box - filled rectangle
Equilateral Triangle
Regular Hexagon
Cone image - Sharp Fuzzy Disc
Hemisphere Image - Dull Fuzzy Disc
Outline shape - you supply coordinates

OK   Cancel

Step-by-step: (9) Select "Box – filled rectangle" which adds a line to the List that will define a rectangle with sides of 20 and 5 pixels located at Position 100 100 tilted 25 degrees from horizontal with intensity 40
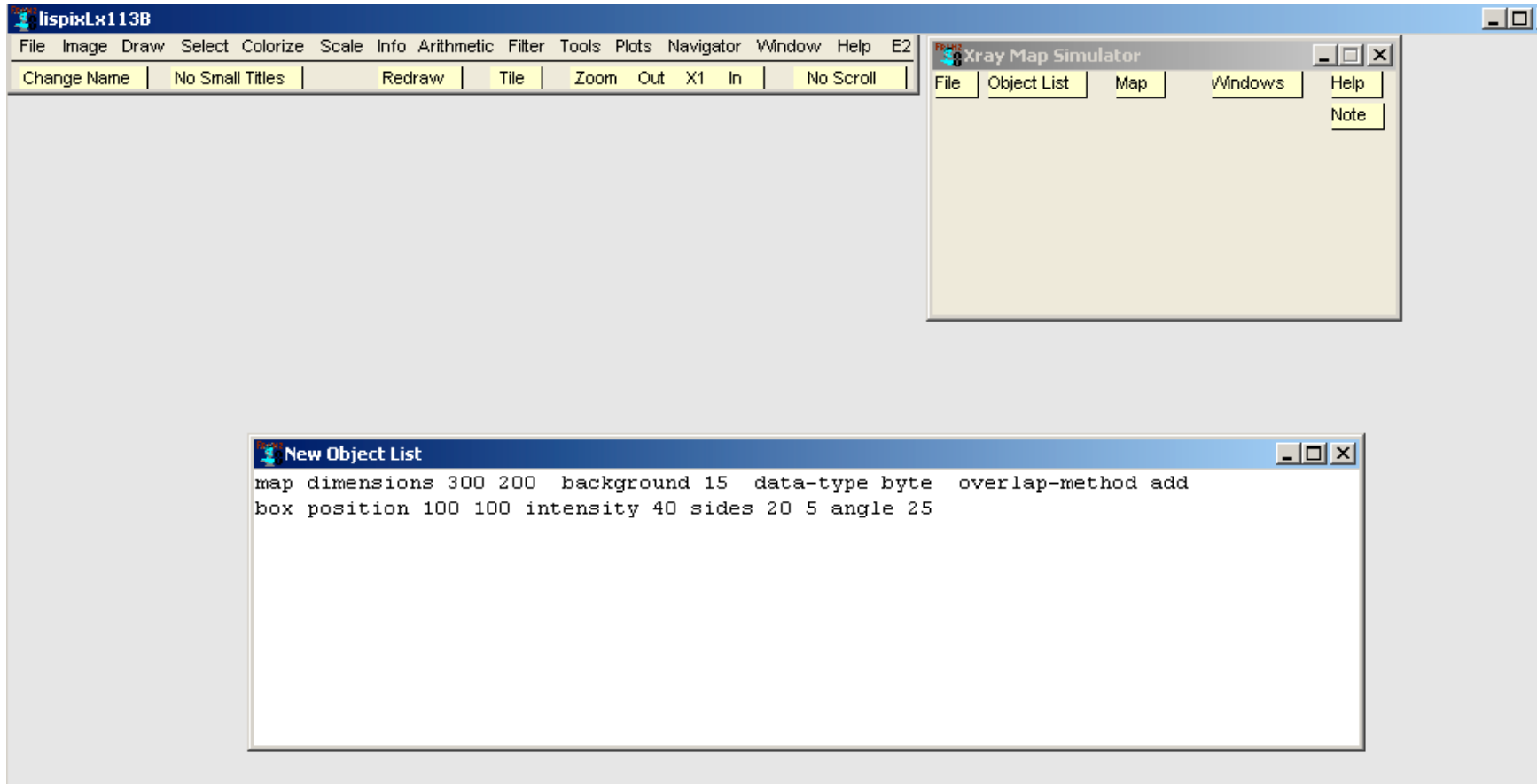
Step-by-step: (10) To see the object specified by these instructions, under "Object List" choose "Make Map"which will produce the image shown giving the template of the map as full white on a black background.
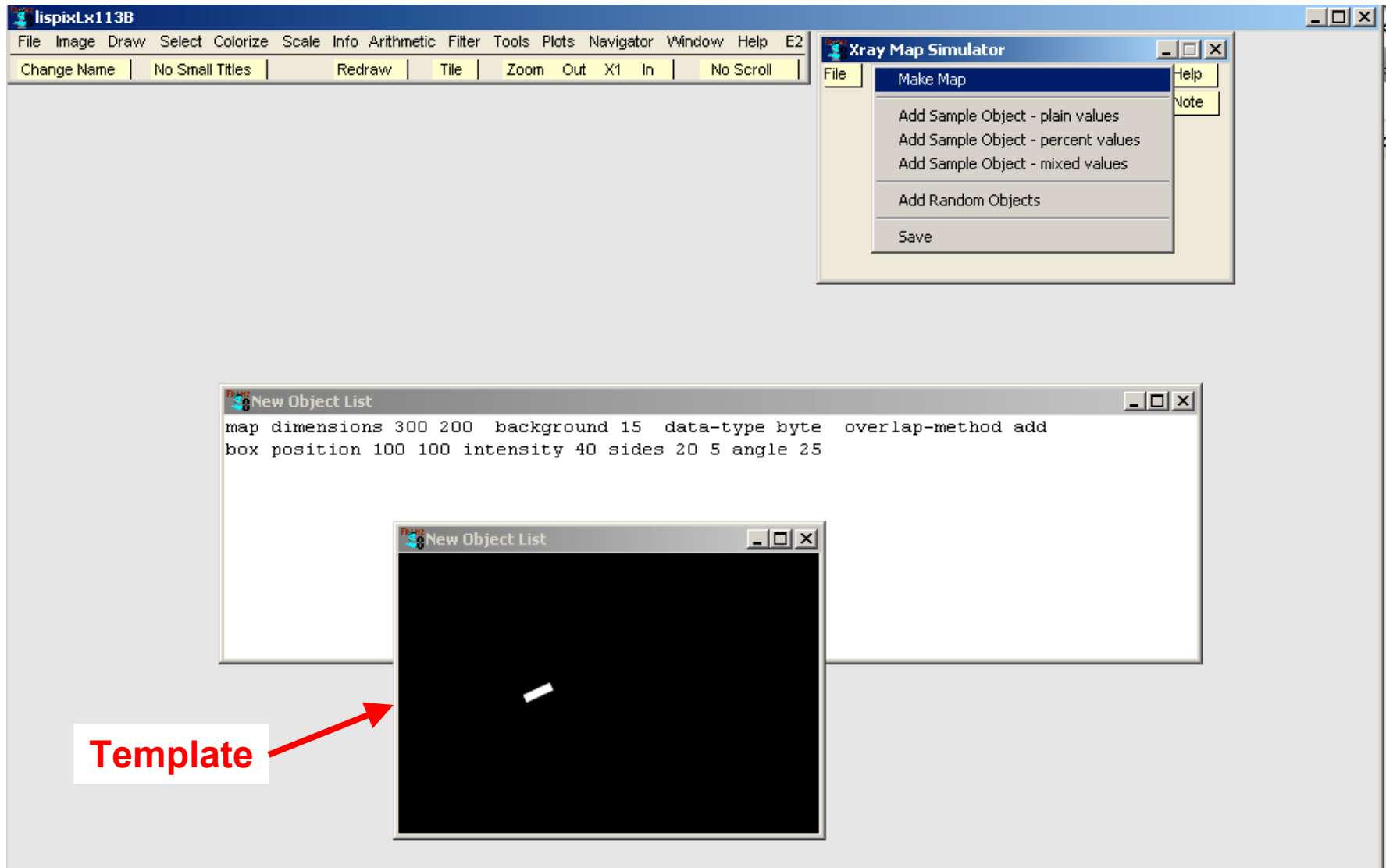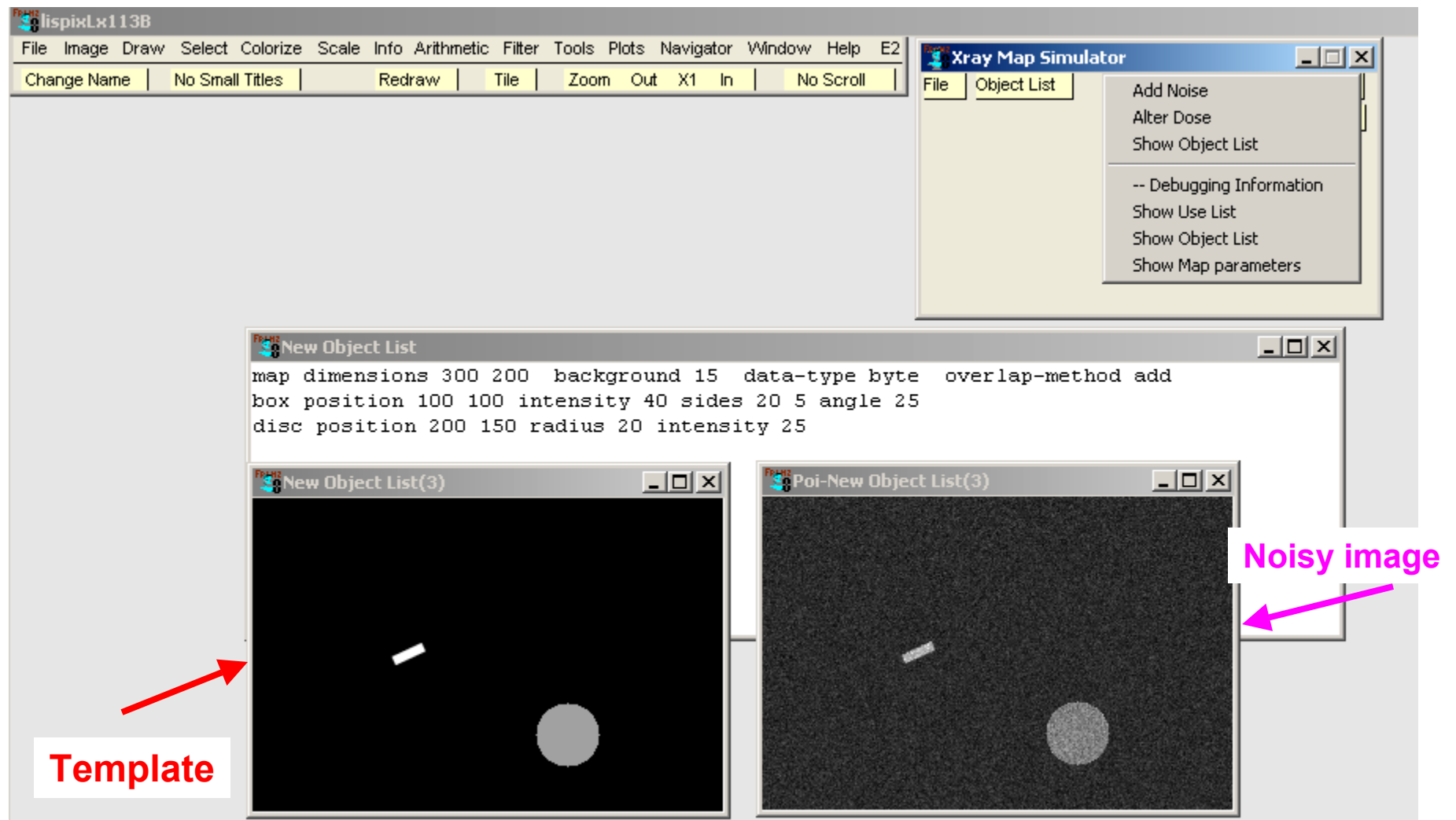

Template

Step-by-step: (11) To see the object with appropriate noise due to counting statistics, under "Map" choose "Add noise""which will produce the image shown next to the template the template.


Template

Noisy image
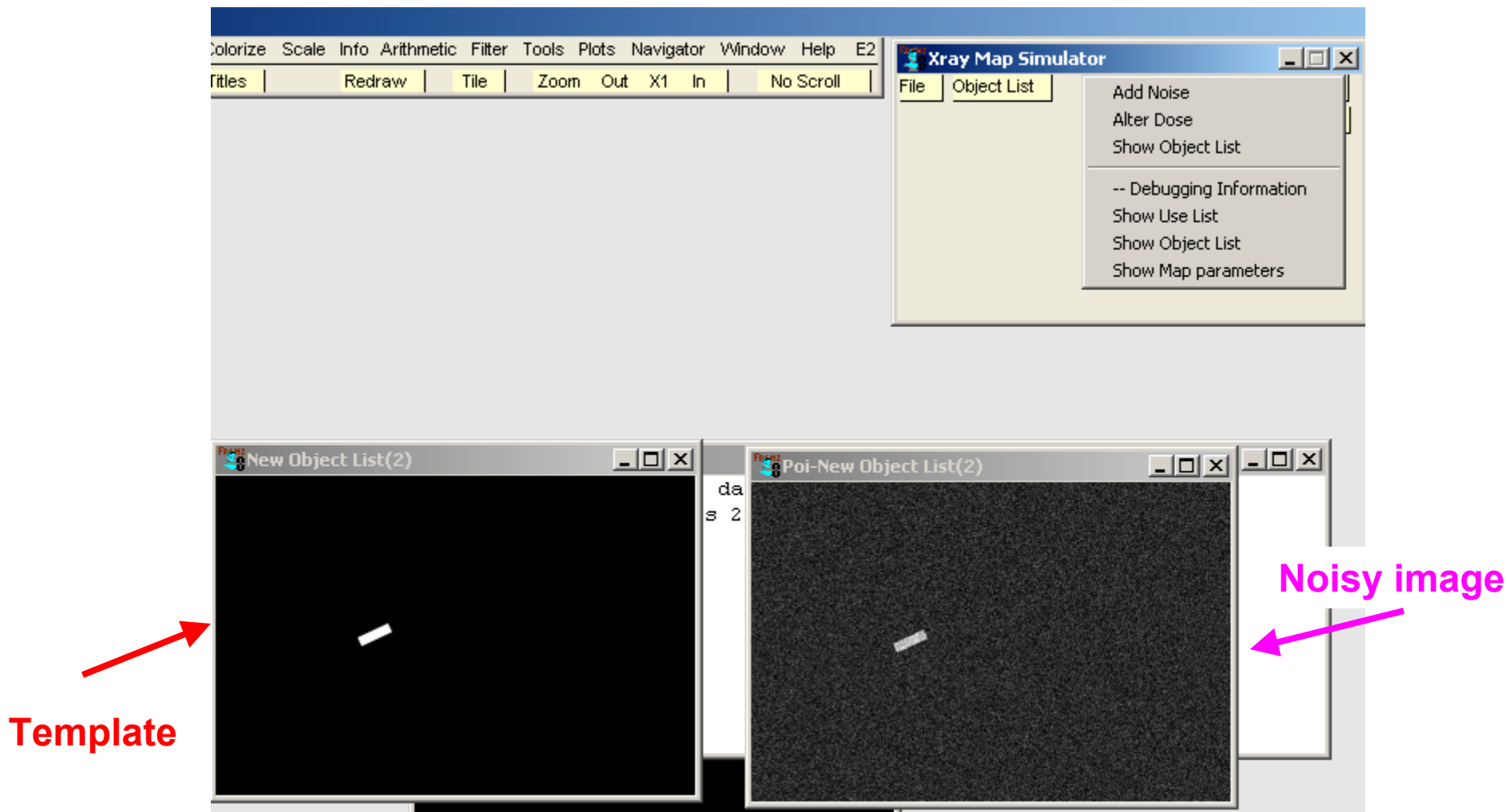
Step-by-step: (12) To add another object, under "Object List" select "Add Sample Object – plain values". This time a disc will be chosen centered At 200 150 with a radius of 20 and intensity 25.
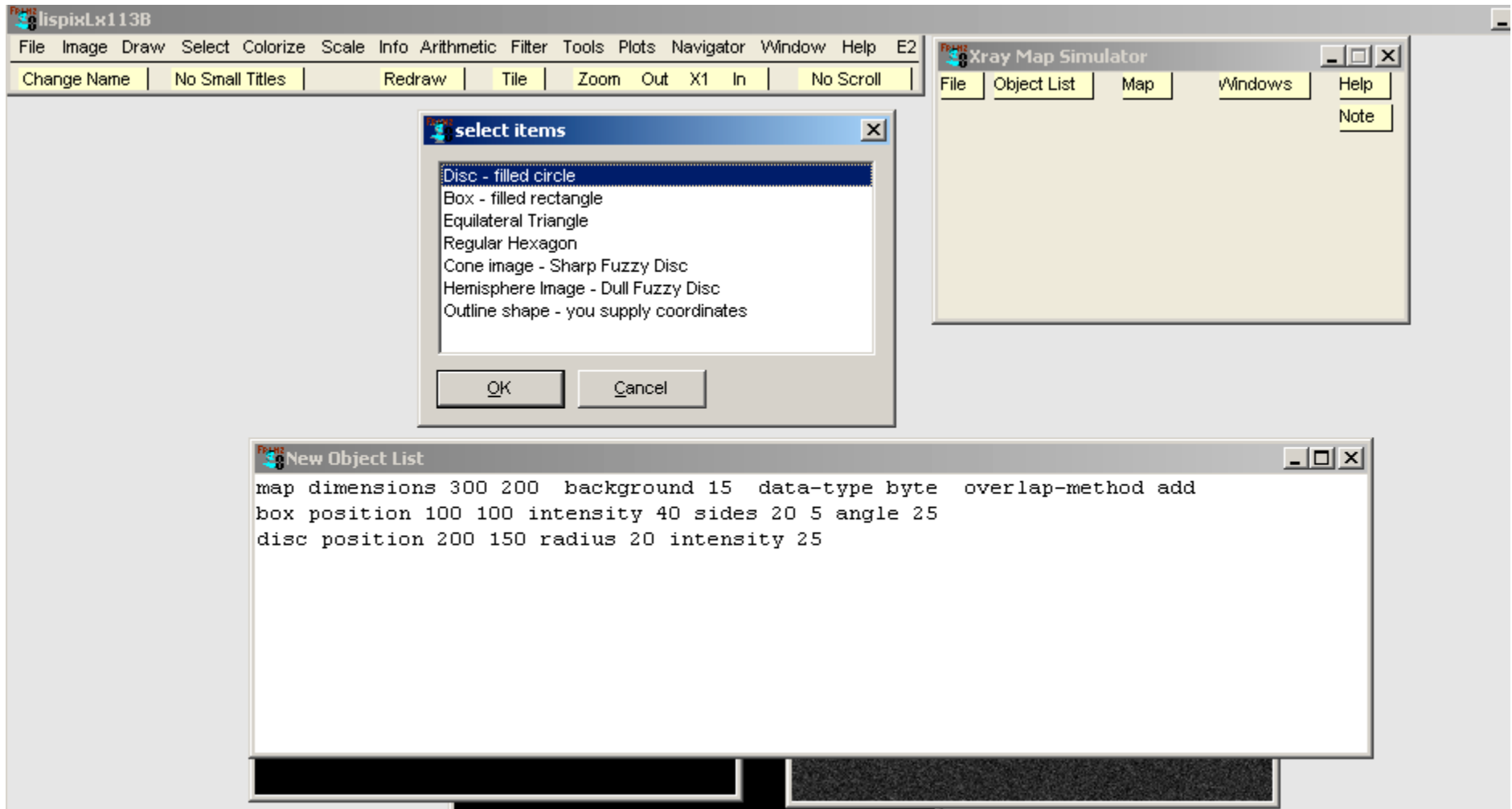
Step-by-step: (13) To see the new template, under "Object List" select "Make Map" and then under Map" select "Add noise" to see final image.

lispixLx113B

File   Image   Draw   Select   Colorize   Scale   Info   Arithmetic   Filter   Tools   Plots   Navigator   Window   Help   E2

Change Name | No Small Titles | Redraw | Tile | Zoom   Out   X1   In | No Scroll |

Xray Map Simulator

File | Object List

Add Noise
Alter Dose
Show Object List

-- Debugging Information
Show Use List
Show Object List
Show Map parameters

New Object List

map dimensions 300 200   background 15   data-type byte   overlap-method add
box position 100 100 intensity 40 sides 20 5 angle 25
disc position 200 150 radius 20 intensity 25

New Object List(3)

Poi-New Object List(3)

Noisy image

Template

Step-by-step: (14) To make a random collection of objects, after creating a new list, under "Object List" choose "Add Random Objects"
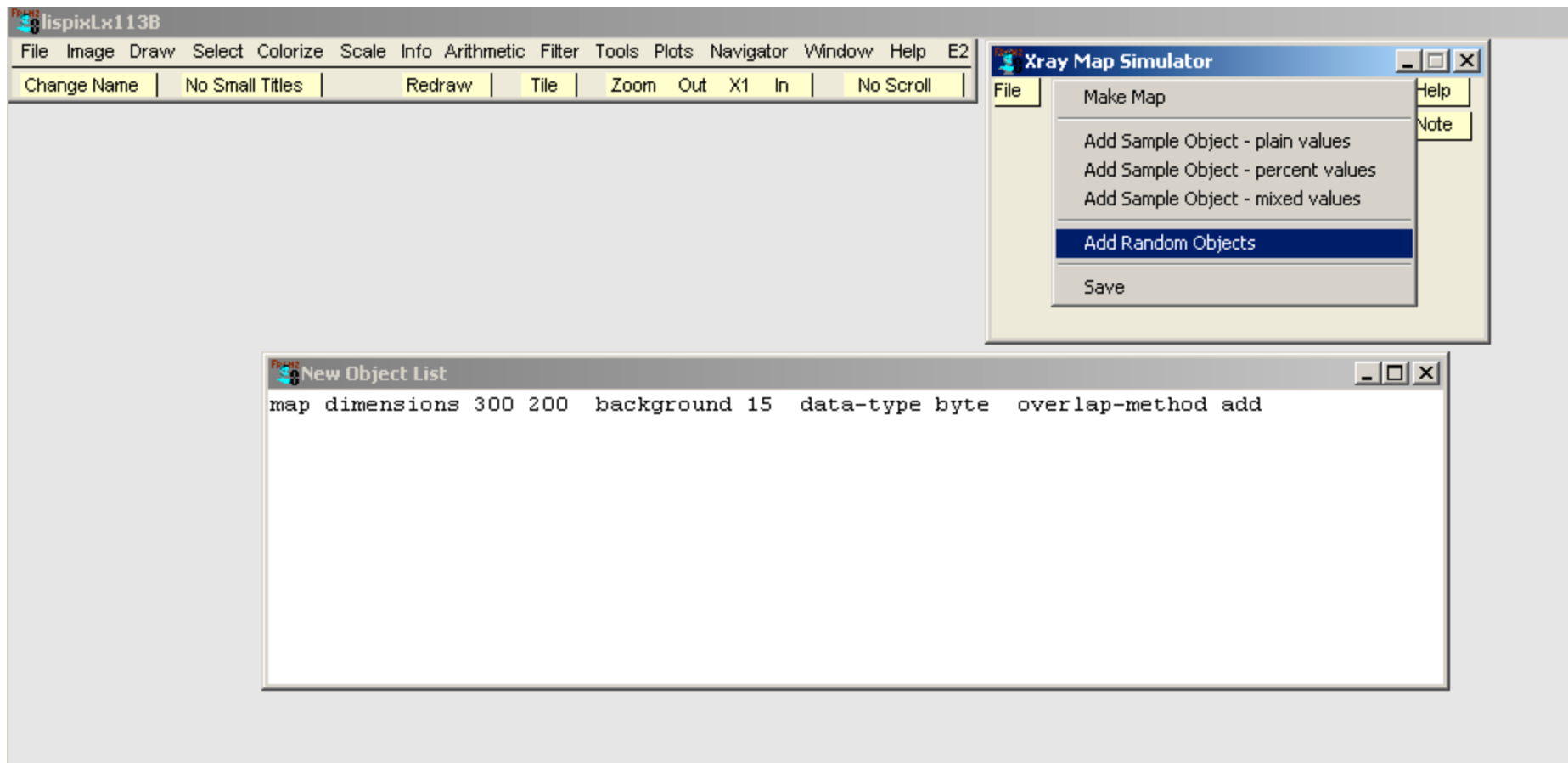
Step-by-step: (15) To make a random collection of objects, after creating a new list, under "Object List" choose "Add Random Objects". A dialogue box will open allowing your choice of discs or boxes
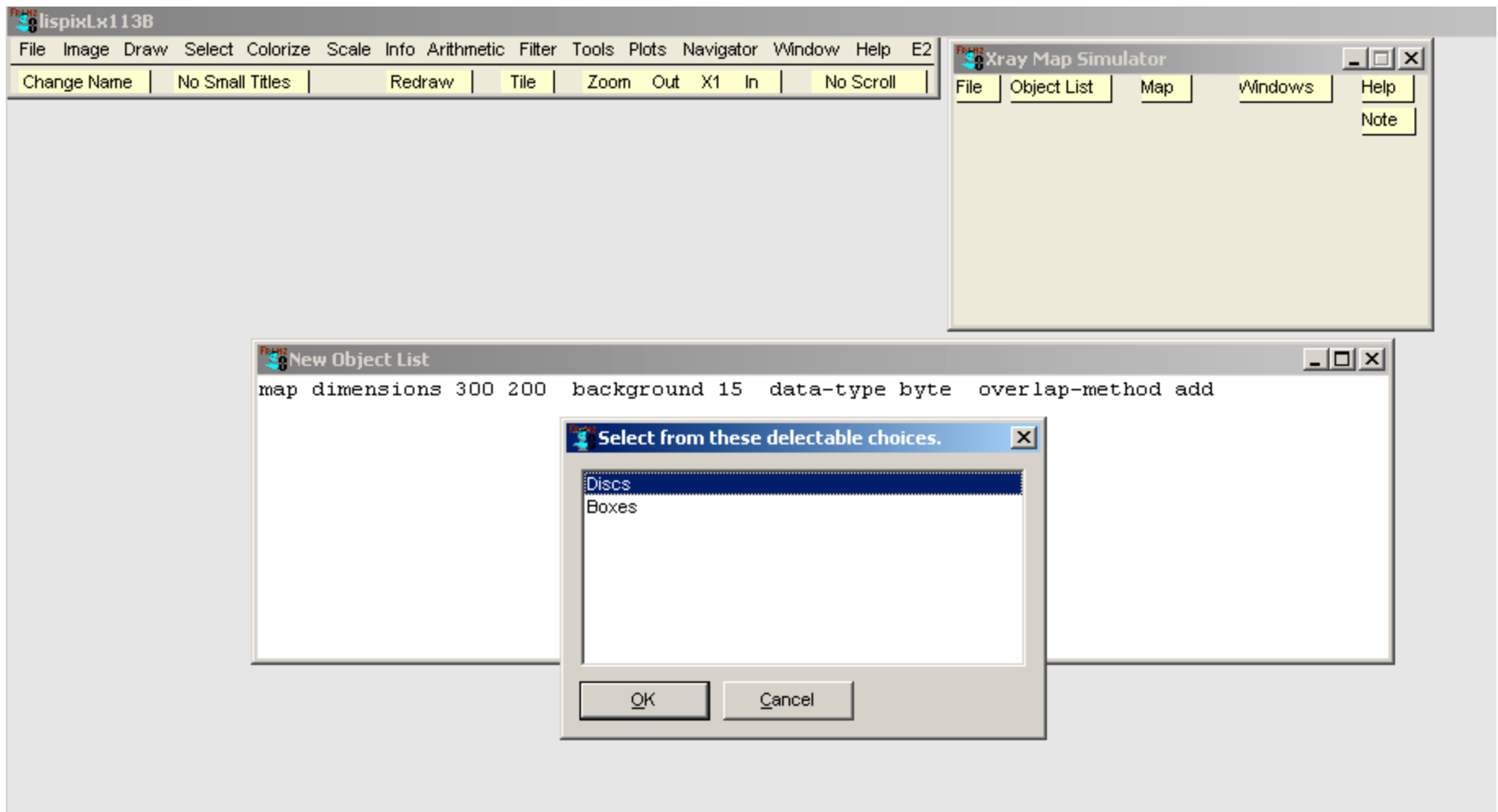
Step-by-step: (16) Next, a dialoguebox will open allowing your choice of the number of objects (default = 5). We have chosen 9 for this example.
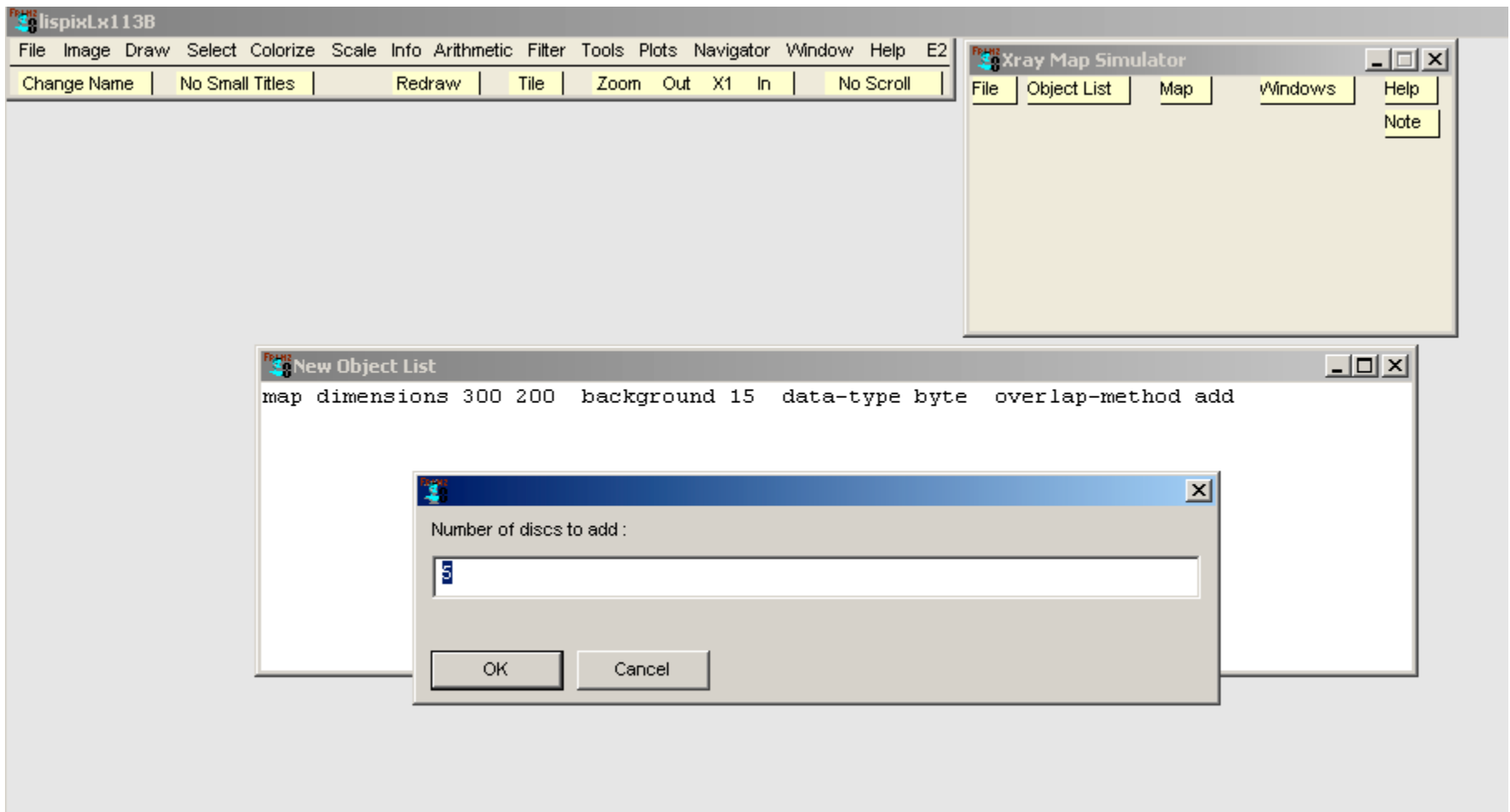
Step-by-step: (17) Next, a dialogue box will open allowing your choice of the size of the objects, e.g., for discs, the range of radii expressed as a percentage of the field width (default = 2% to 10%).
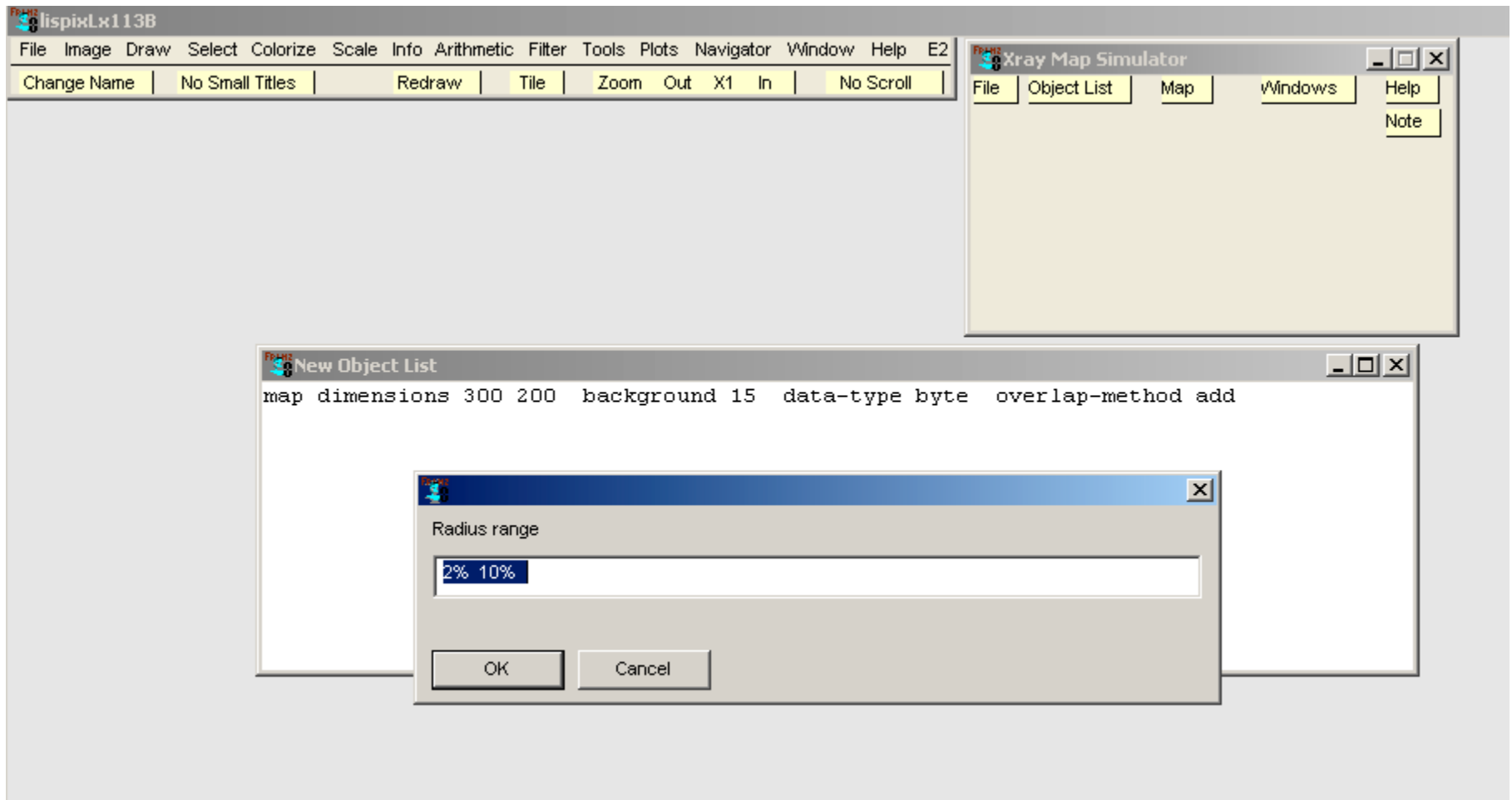
Step-by-step: (18) Next, a dialogue box will open allowing your choice of the intensity range relative to the background for the objects, e.g., (default = 70% to 200%).
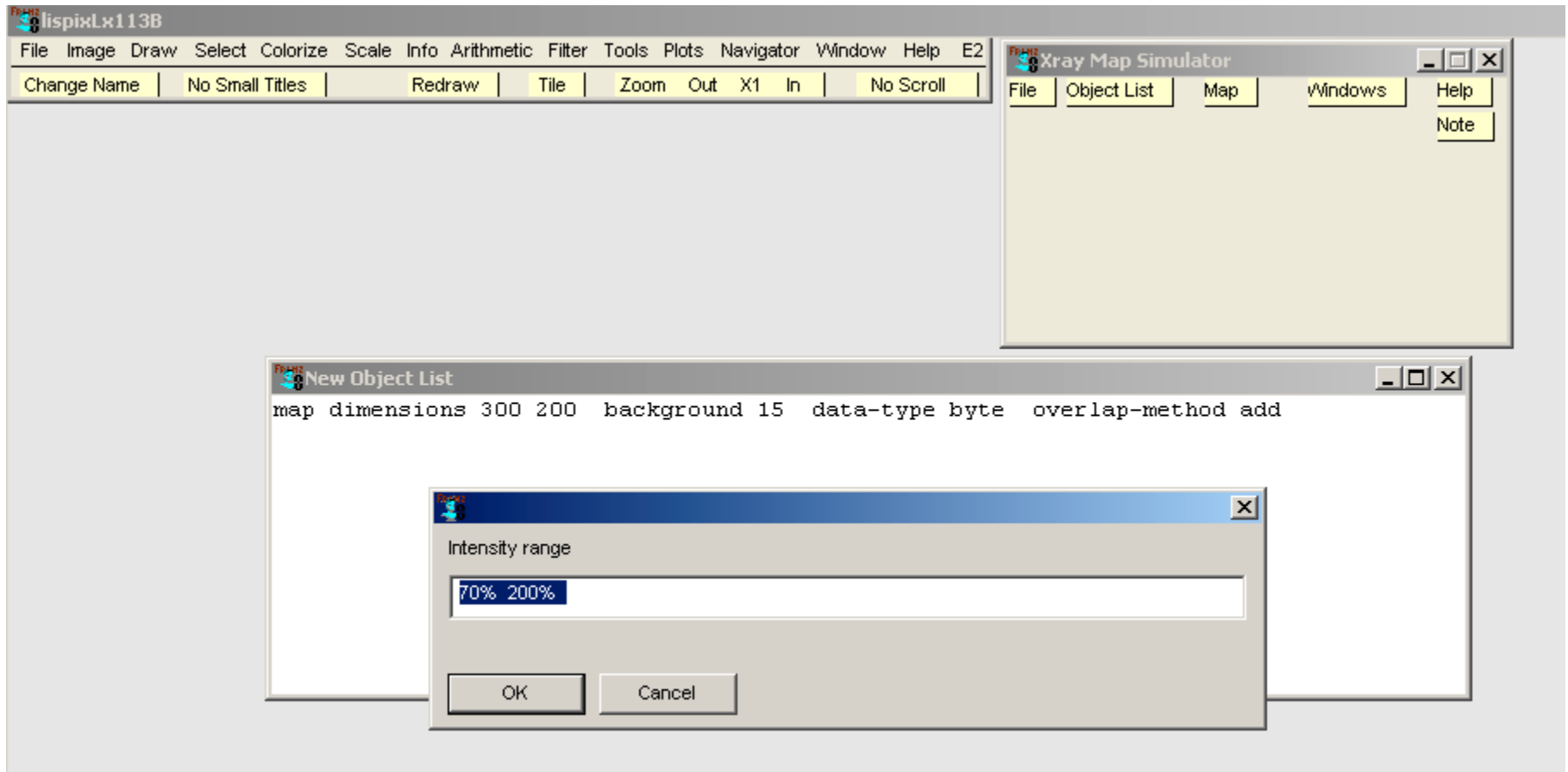
Step-by-step: (19) The list of random objects will be written. If any of them intersect the boundary of the frame, a warning message will appear.
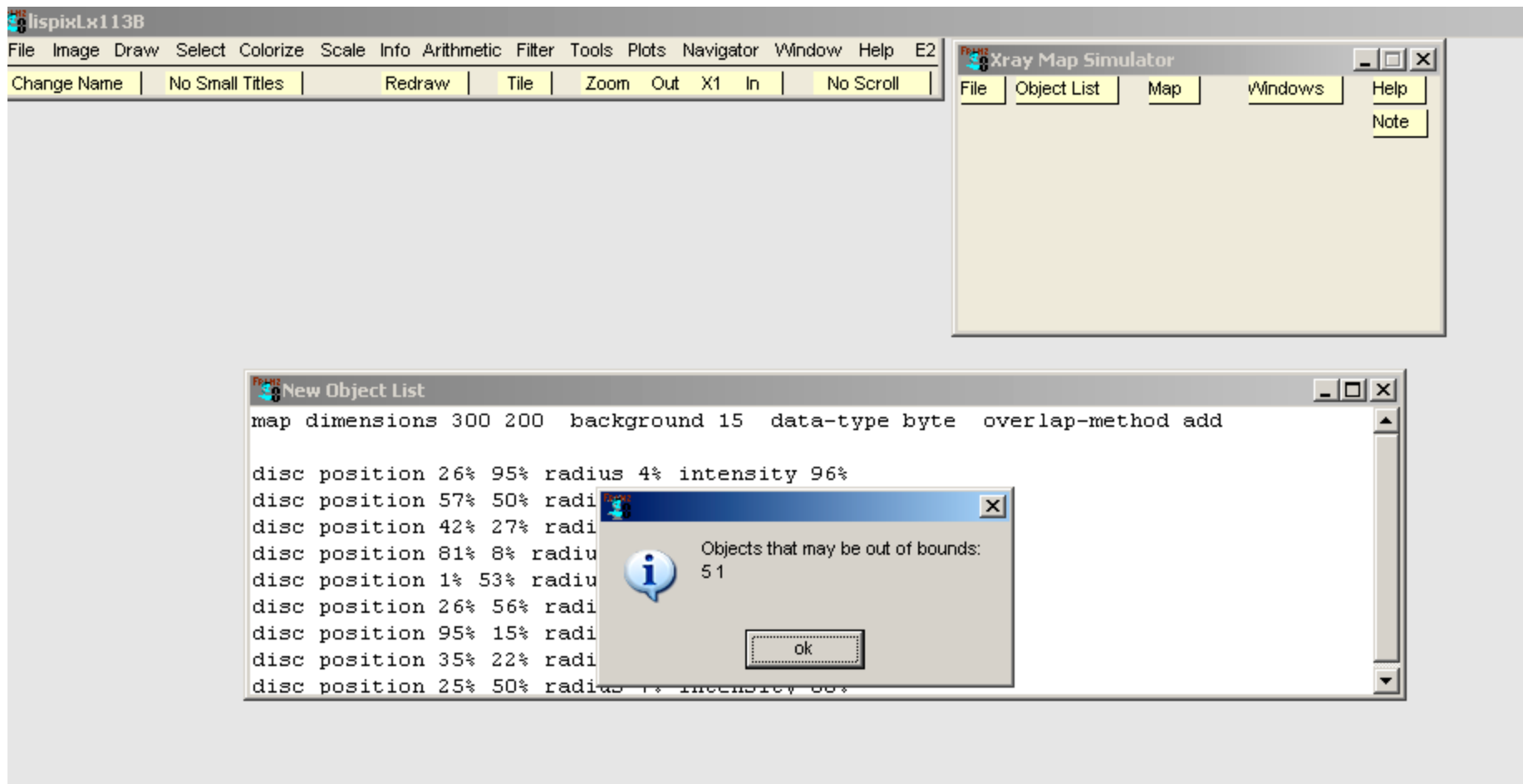
Step-by-step: (20) To see the results, under "Object List" choose "Make Map" and under "Map" choose "Add Noise".