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INTERPRETATION AND DISPLAY OF THE NURE DATA BASE USING COMPUTER GRAPHICS

by

Dr. Glenn R. Koller

E. I. du Pont de Nemours & Co.
Savannah River Laboratory
Aiken, SC 29808

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Dr. Glenn R. Koller
E. I. du Pont de Nemours & Co.
Savannah River Laboratory
Aiken, SC 29808
USA
(803) 725-3481

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NURE PROGRAM OBJECTIVES

The National Uranium Resource Evaluation (NURE) program was established by the U. S. Department of Energy in 1973. The primary objective of the NURE program is to assess the nation's recoverable uranium reserves. To this end, Savannah River Laboratory (SRL), operated by E. I. du Pont de Nemours & Co., has accepted responsibility to collect and analyze water and sediment samples and to report geochemical analyses of the samples from 30 eastern and 7 western states (Figure 1). Oak Ridge Gaseous Diffusion Plant and Los Alamos Scientific Laboratory have accepted similar responsibilities in the remaining contiguous states and Alaska.

TECHNICAL BASIS FOR THE NURE PROGRAM

SRL is collecting sediment, ground water, and stream water samples in its 3.9 million km^2 (1.5 million mi^2) area of responsibility at a target density of one sample per 15.6 km^2

* Work done under USDOE contract No. DE-AC09-76SR00001.

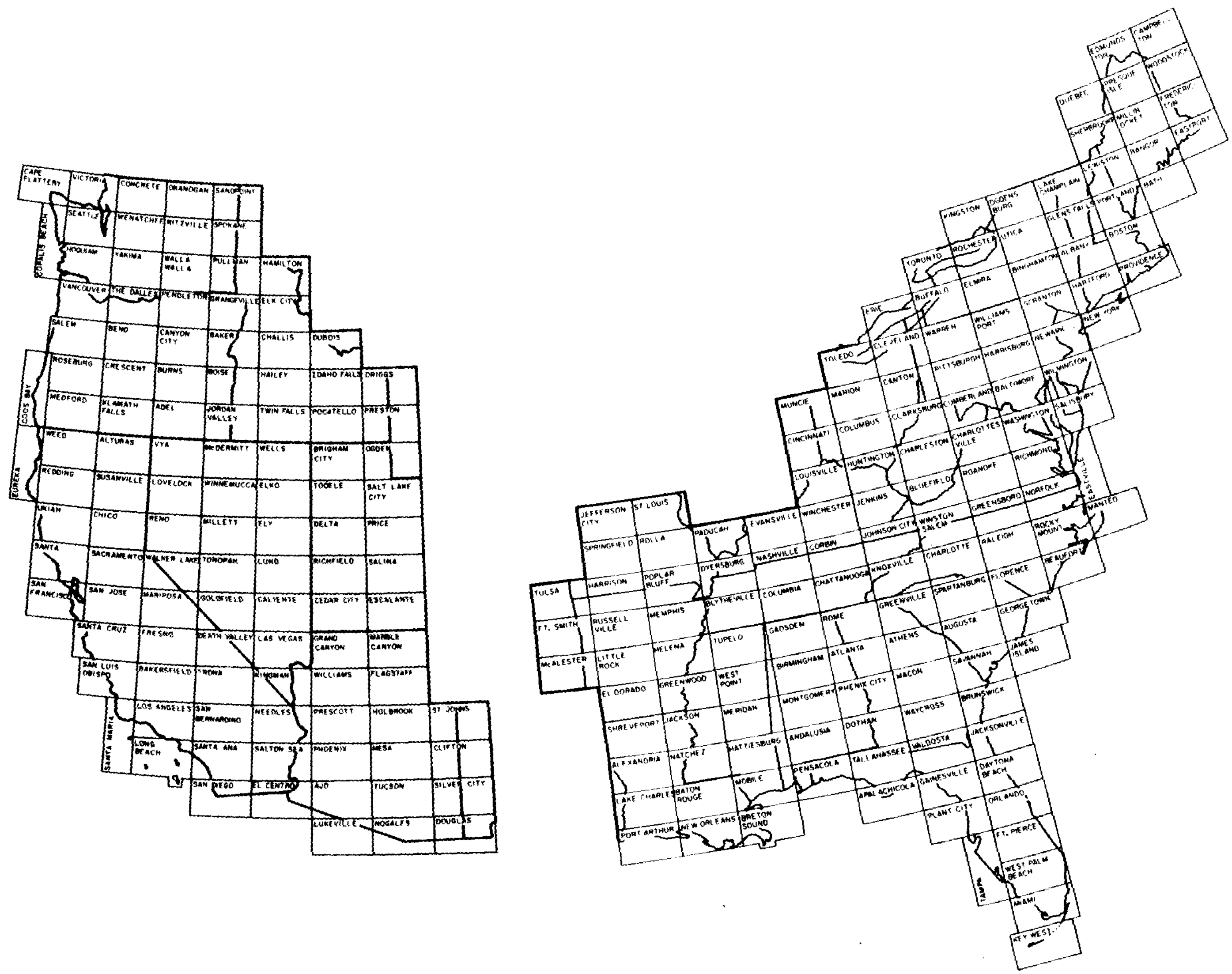


FIGURE 1. SRL area of responsibility.

(6 mi^2) using sample collection techniques developed at SRL (Price and Jones, 1979). Stream sediments are the primary non-aqueous samples collected in the eastern U. S. Surface sediment (soils) are dominant in the west. Analytical techniques such as neutron activation (Hochel, et al., 1980), x-ray fluorescence, laser fluorescence, atomic absorption, and other methods are used to determine the concentrations of 39 elements in sediment samples and 37 elements in water samples (Table 1). In addition to elemental data, site-specific field data are collected for each sample (Table 2).

COMPUTING FACILITIES AND GRAPHICS CAPABILITIES

The in-house data processing facility utilized by SRL primarily consists of an IBM 370/155 and an IBM 360/195. The primary graphics device used by the NURE program, in addition to high-speed printers, is the Information International Inc. FR80. Coding for the NURE program at SRL primarily is in SAS (SAS Users Guide, 1979) and FORTRAN IV. Graphics packages used, and to be discussed here, include DISSPLA (DISSPLA Manual, Vol I, 1973), Surface II (Sampson, 1975), and TELL-A-GRAF (TELL-A-GRAF Reference Manual, 1978).

Samples are collected, processed, and reported in $1^\circ \times 2^\circ$ National Topographic Map Series (NTMS) units (Figure 1). Within the bounds of each quadrangle, on the average, 1200 sediment and 500 stream water and ground water samples are collected.

Concentrations Are Determined for the Following Elements in Sediments:

Ag, Al, As, Ba, Be, Ca, Ce, Co, Cr, Cu, Dy, Eu, Fe, Hf, K, La, Li, Lu, Mg, Mn, Mo, Na, Nb, Ni, P, Pb, Sc, Se, Sm, Sn, Sr, Ti, Th, U, U (extractable), V, W, Y, Yb, and Zn.

Concentrations Are Determined for the Following Elements in Water Samples:

Ag, Al, As, B, Ba, Be, Br, Ca, Ce, Cl, Co, Cr, Cu, Dy, F, Fe, He, K, Li, Mg, Mn, Mo, Na, Nb, Ni, P, Sc, Se, Si, Sr, Ti, Th, U, V, Y, Zn, and Zr.

Field Measurements and Observations Taken at Sampling Sites:

ADDRESS	ROCK TYPE
ALKALINITY	SAMPLE TYPE
CONDUCTIVITY	SCINTILLOMETER READING
CONFIDENCE OF WELL DEPTH	SEDIMENT SIZE
CONTAMINANTS	STATE
DATE	STREAM DEPTH
FORMATION	STREAM FLOW
DEPTH OF WELL	STREAM LEVEL
NUMBER OF COMPOSITES	STREAM WIDTH
ODOR	TEAM NUMBER
pH	VEGETATION DENSITY
RELIEF	VEGETATION TYPE

Analysis of these samples for the elements listed in Table 1 generates a data base of approximately 89,000 analyses for each $1^{\circ} \times 2^{\circ}$ quadrangle. A data base of about 21,000,000 elemental analyses is expected when all samples are analyzed from the 238 quadrangles which comprise SRL's area of responsibility. Field data (Table 2) collected at each sampling site add significantly to the size and complexity of the data base.

It is the charge of NURE geologists to integrate the known geology of an area with elemental and field data in order to identify areas favorable for recovery of uranium. Manual manipulation of single or multiple data sets (quadrangles), considering the constraint of time, is impractical. NURE geologists at SRL, therefore, have employed a variety of statistical and computer-graphics techniques to aid in the interpretation of hydrogeochemical data.

The most straight-forward method of interpretation of areally distributed geochemical data is that of generating a contour map. Figure 2 is a contour map of log U/Hf values in the Portland $1^{\circ} \times 2^{\circ}$ NTMS quadrangle. Ratios and logs were calculated in a SAS routine and passed to SURFACE II for plotting. Using SAS data set storage techniques on resident disks, separate data sets can be concatenated and considered as a single unit for plotting as in Figure 3. Figure 3 is a

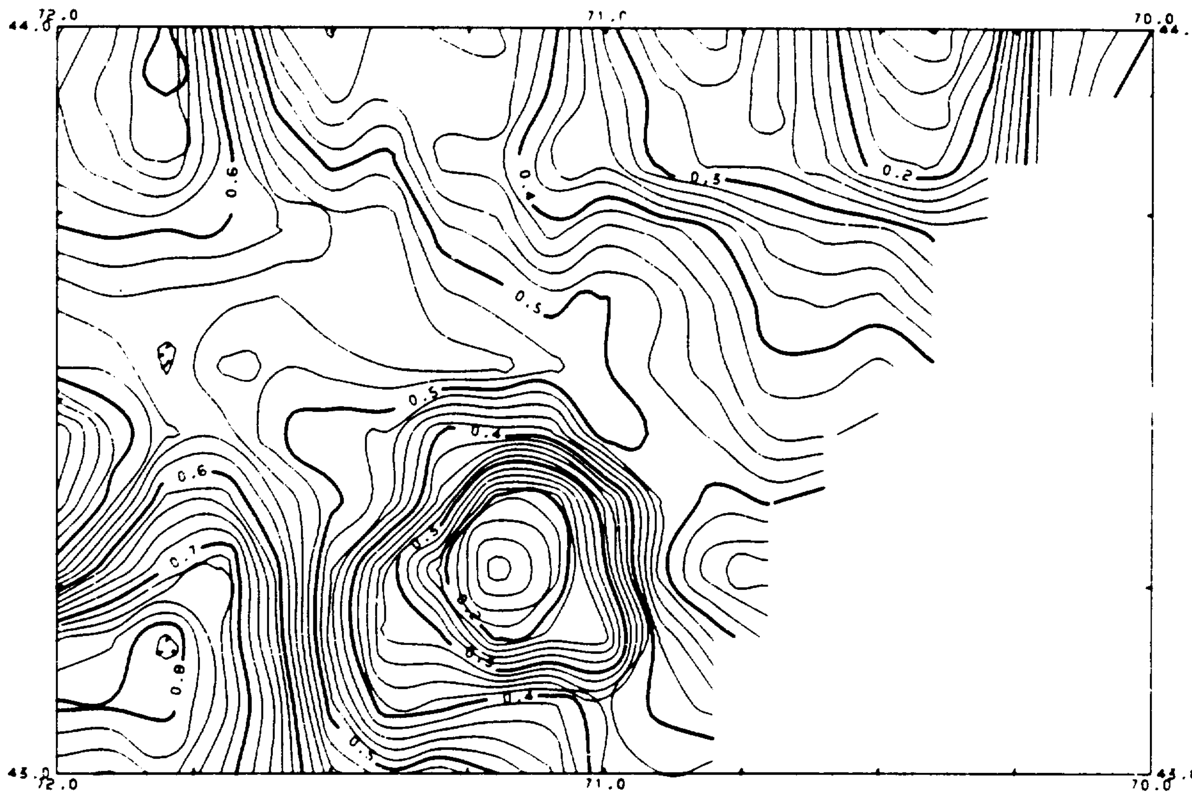


FIGURE 2. SURFACE II contour map of log U/Hf in the Portland 1° x 2° NTMS quadrangle. Eastern portion of map is Atlantic Ocean.

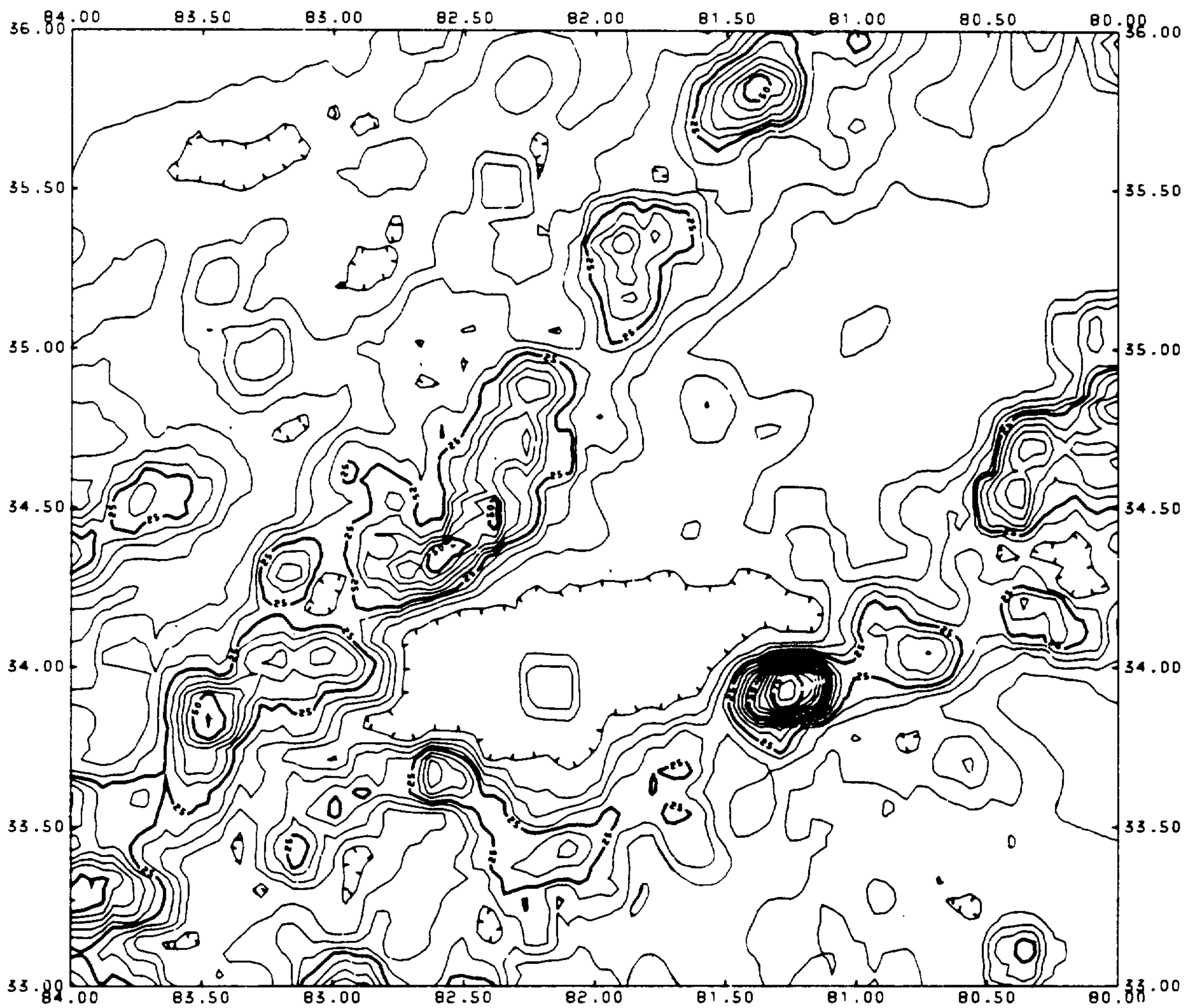


FIGURE 3. SURFACE II contour map of uranium in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles.

compilation of data from the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles. The contrast between Figures 2 and 3 in the "smoothness" of the contour lines is a result of choosing different grid and smoothing options offered by SURFACE II and reflects well the flexibility of this graphics package. Three-dimensional plots also can be created using SAS and SURFACE II (Figure 4). As can be seen by comparing Figures 3 and 4, linear trends and relative magnitudes are more easily perceived in a three-dimensional plot.

Combining FORTRAN IV and SAS software with the graphics capabilities of SURFACE II allows SRL-NURE geologists to concatenate single data sets and then to "window" selected data. The "window" process can be accomplished in two ways. In Figure 5, residual uranium values were calculated by a SAS regression routine for the entire area enclosed by the rectilinear boundary of the plot. SURFACE II commands, however, permit the display, for example, of only those data in northwestern South Carolina. This method of "windowing" allows SRL geologists to display select data without sacrificing the relationship of the displayed data to those not depicted.

A second method used to display subsets of data is demonstrated by the posting or "spot map" of Figure 6. A FORTRAN IV routine was used to separate those data within the

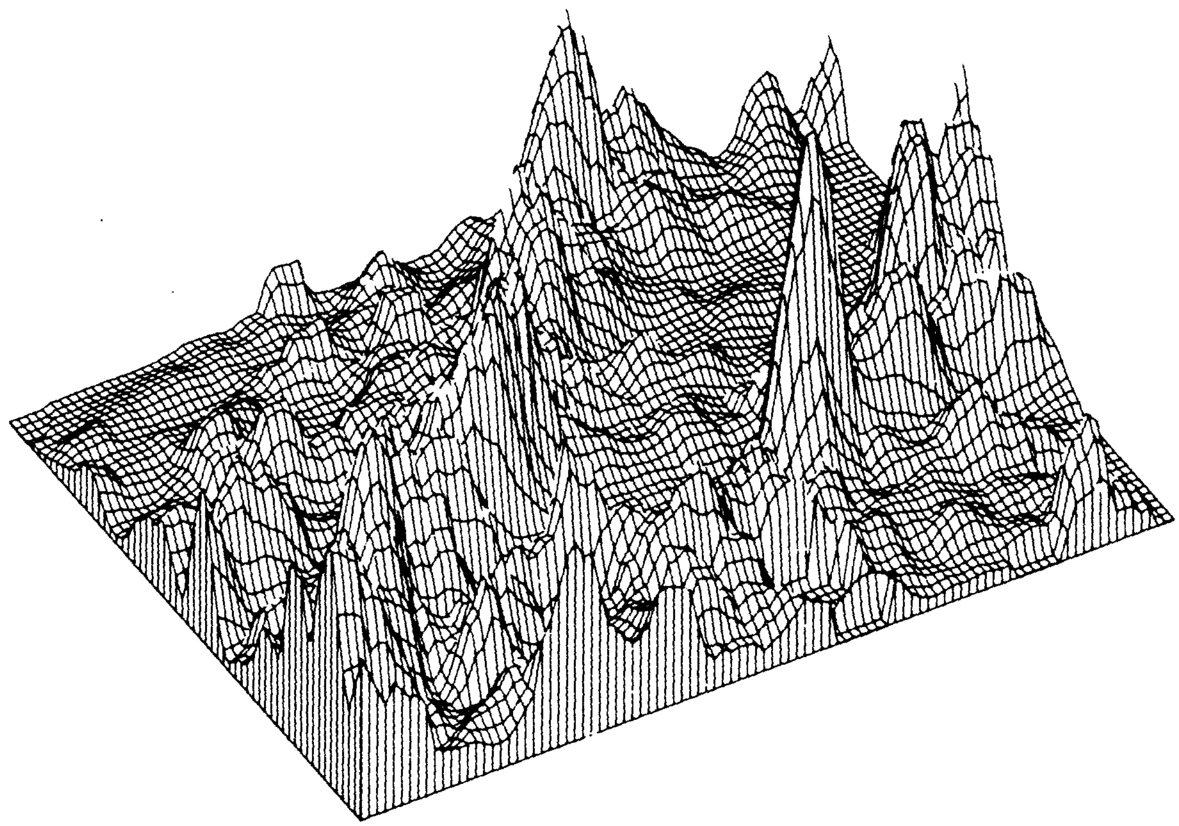


FIGURE 4. SURFACE II three-dimensional plot of uranium in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles.

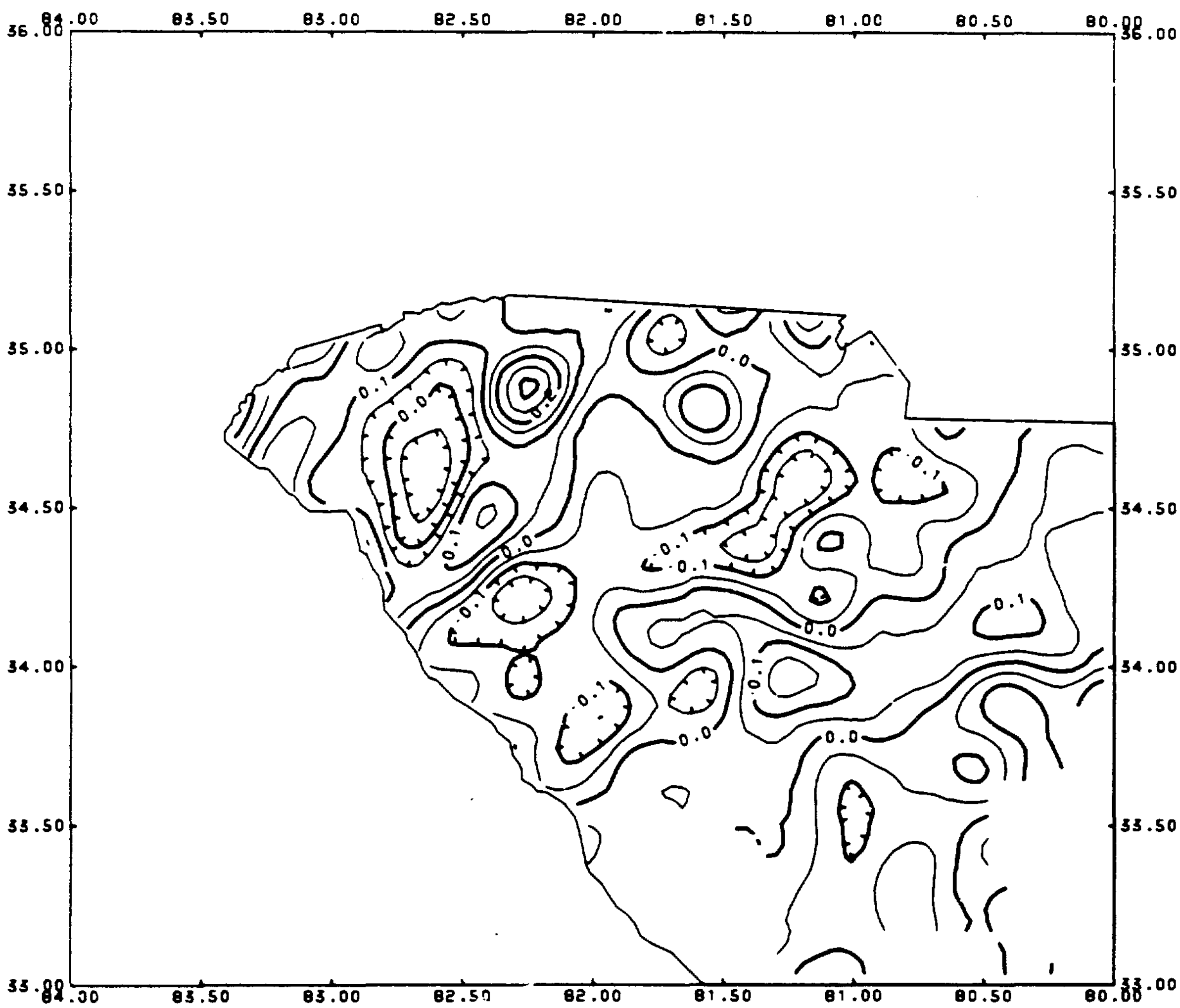


FIGURE 5. Contour map of residual uranium values in central and western South Carolina.

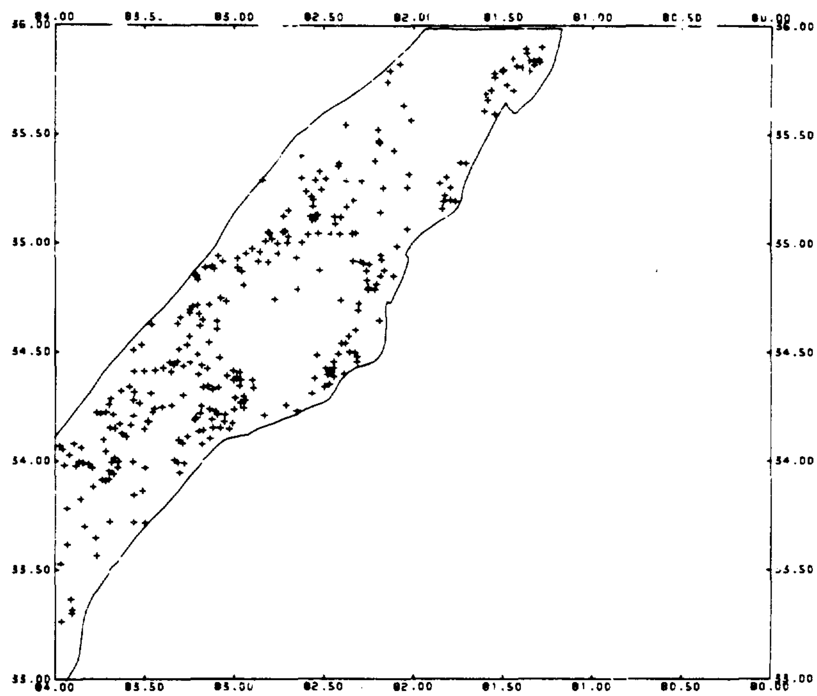
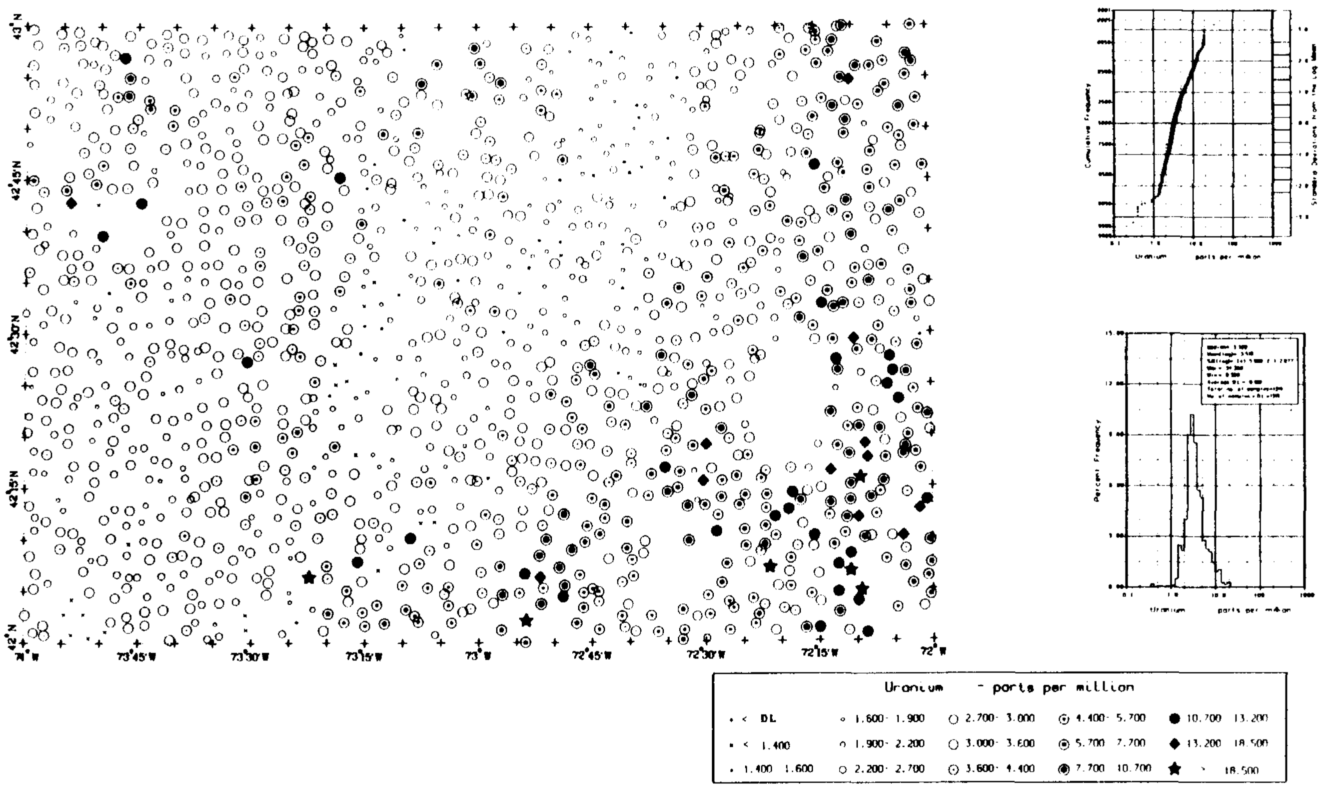


FIGURE 6. Posting of sample sites from which calculated uranium residual values are greater than 0.15.

irregular bounds of part of the Piedmont, a geologic province east of the Appalachian Mountains, and to store those data as a separate file. This method of "windowing" permits the compilation of statistics on only those data within a subset. Figure 6 was produced using SAS to filter calculated residual uranium values so that only those values greater than 0.15 were plotted by SURFACE II.

A more sophisticated technique for the display of areally distributed data is shown in Figure 7. The DISSPLA computer graphics package was used to combine an areal distribution symbol-plot map with a histogram and a cumulative frequency plot of uranium data from the Albany $1^{\circ} \times 2^{\circ}$ NTMS quadrangle. The symbol-plot map, unlike the contour map, yields information concerning individual samples (each symbol represents a single sediment sample) and makes evident which areas and samples have relatively high concentrations of the element in question.

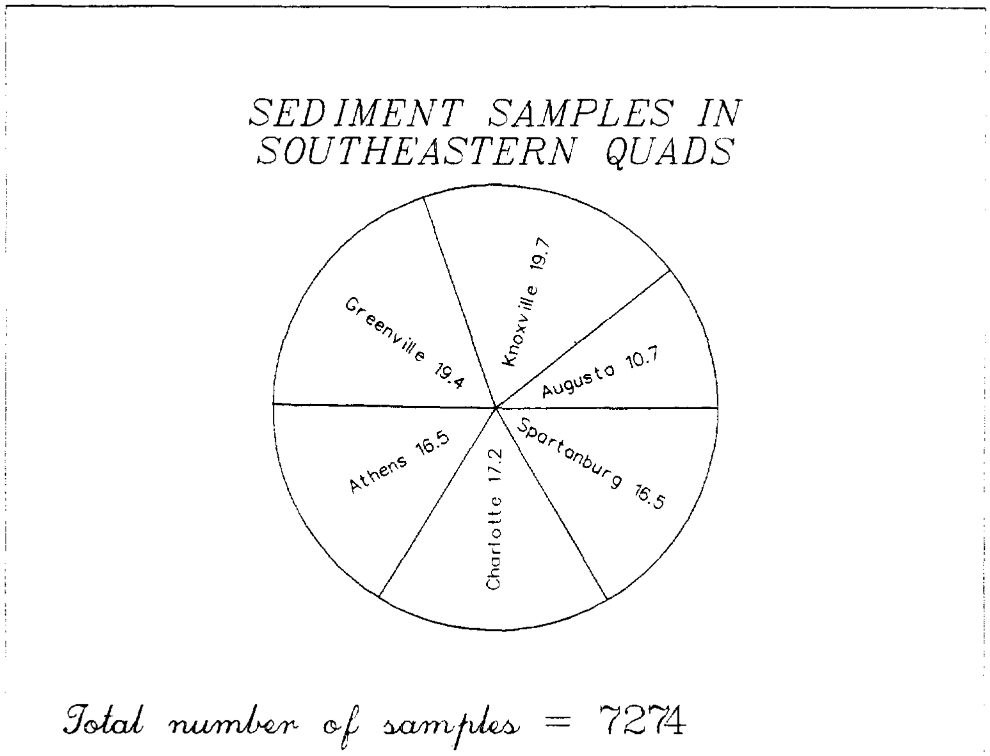
Figure 8 demonstrates the ability of the TELL-A-GRAF graphics system to summarize and report data. The versatility of TELL-A-GRAF software makes it ideal for presenting voluminous technical data to non-technical audiences.

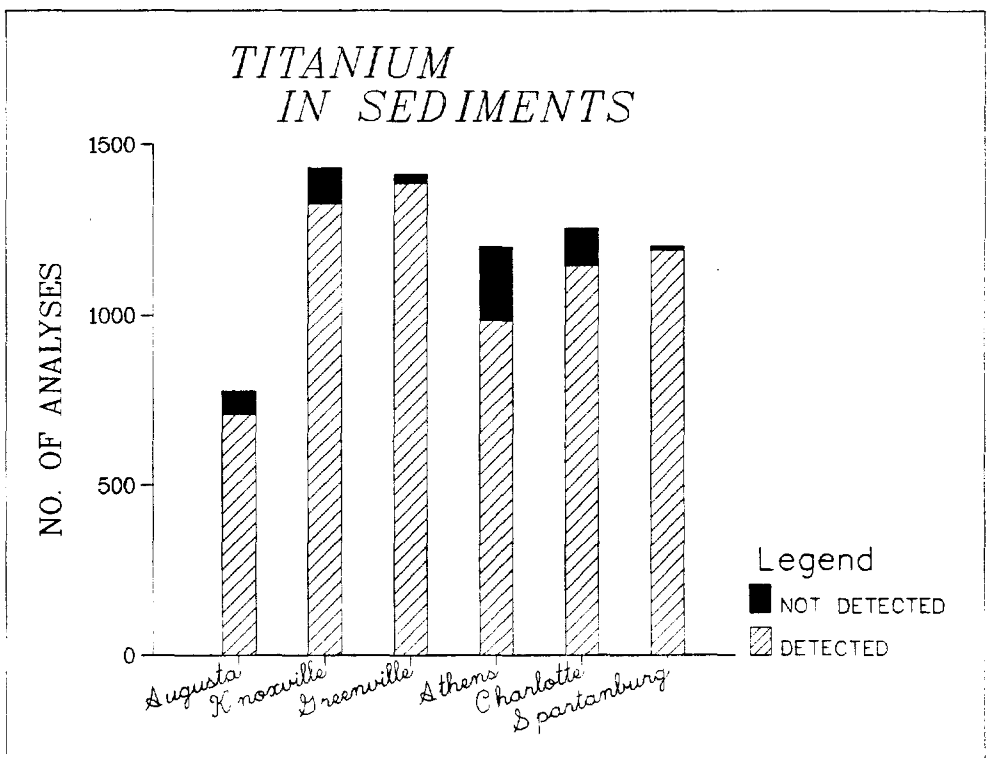


URANIUM DISTRIBUTION IN THE SEDIMENTS

PLATE 5 OF THE *ALBANY* QUADRANGLE

FIGURE 7. DISSPLA plot including an areal distribution symbol-plot map, a histogram, and a cumulative frequency plot of uranium values in the Albany 1° x 2° NTMS quadrangle.





FIGURES 8a and 8b. TELL-A-GRAF plots summarizing hydrogeochemical data.

APPLICATIONS OF COMPUTER GRAPHICS TO NURE DATA

The primary charge of the NURE geologic group at SRL is to correlate field, elemental, and (in special cases) geophysical data with the geology of a given area. Figure 9 is a three-dimensional model of the subsurface configuration of a granitic pluton in the northeastern U. S. based upon gravity and magnetic data. Data for Figure 9 were collected and modeled by the author prior to his involvement in the NURE program.

Two-dimensional models of geophysical data were calculated (Talwani, 1959) and integrated using SURFACE II to produce the models in Figure 9. Three-dimensional representation of potentially economic geologic units can be instrumental in estimating the total reserves of a commodity represented by the unit. In the case of Figure 9, the pluton has a calculated volume of approximately 1460 km^3 (350 mi^3).

Three-dimensional models also are of benefit when the chemical signatures of geologic units are sought. Figure 10 is a three-dimensional plot of hafnium concentrations in the Charlotte $1^{\circ} \times 2^{\circ}$ NTMS quadrangle. Rock units in the quadrangle readily are identified by their hafnium content. Series of such three-dimensional plots in conjunction with geologic maps are used by SRL-NURE geologists to geochemically characterize geologic units.

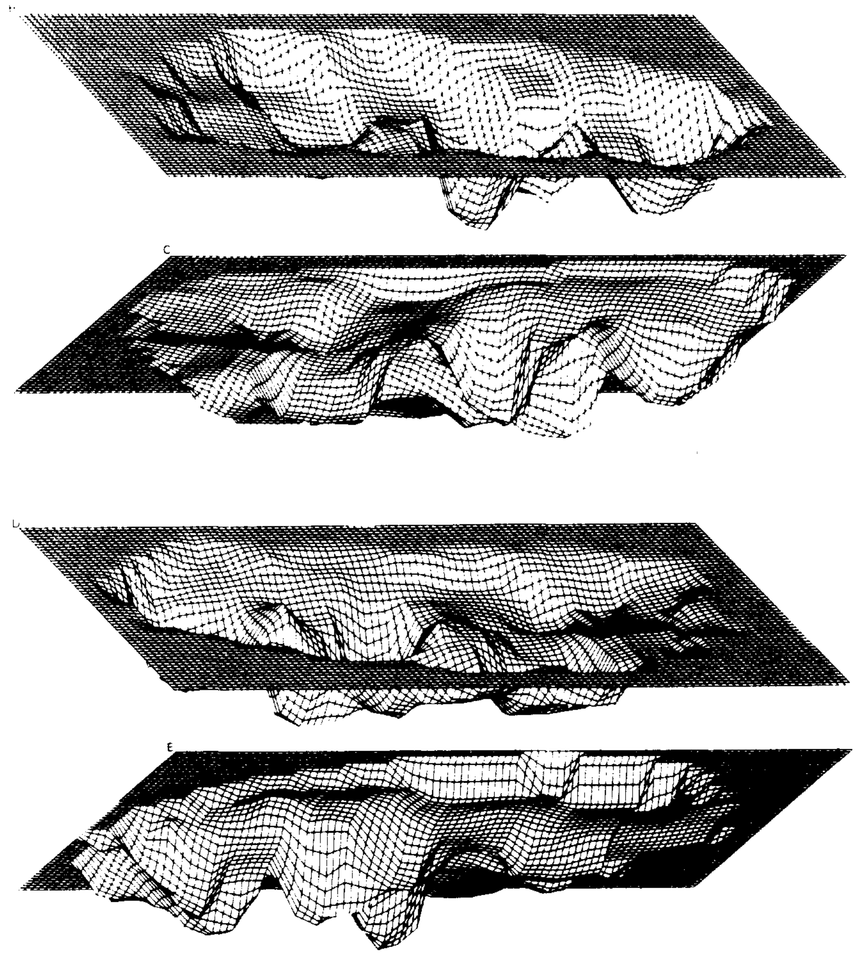


FIGURE 9. Three-dimensional plots of the subsurface distribution of a granitic pluton. Model is based upon geophysical data.

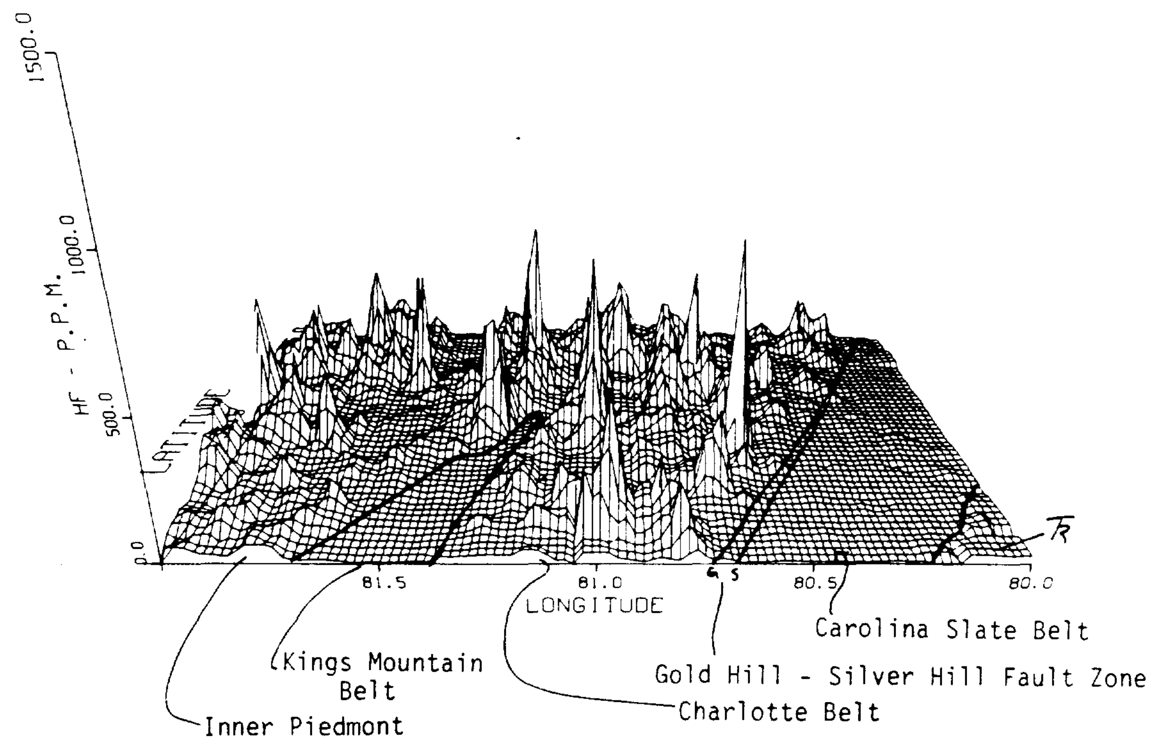
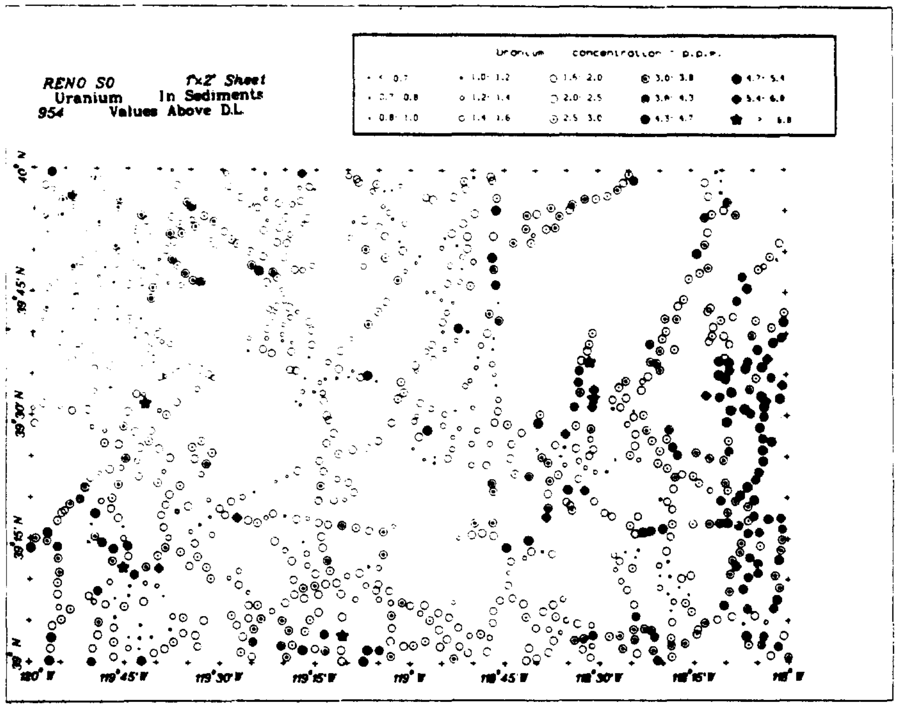
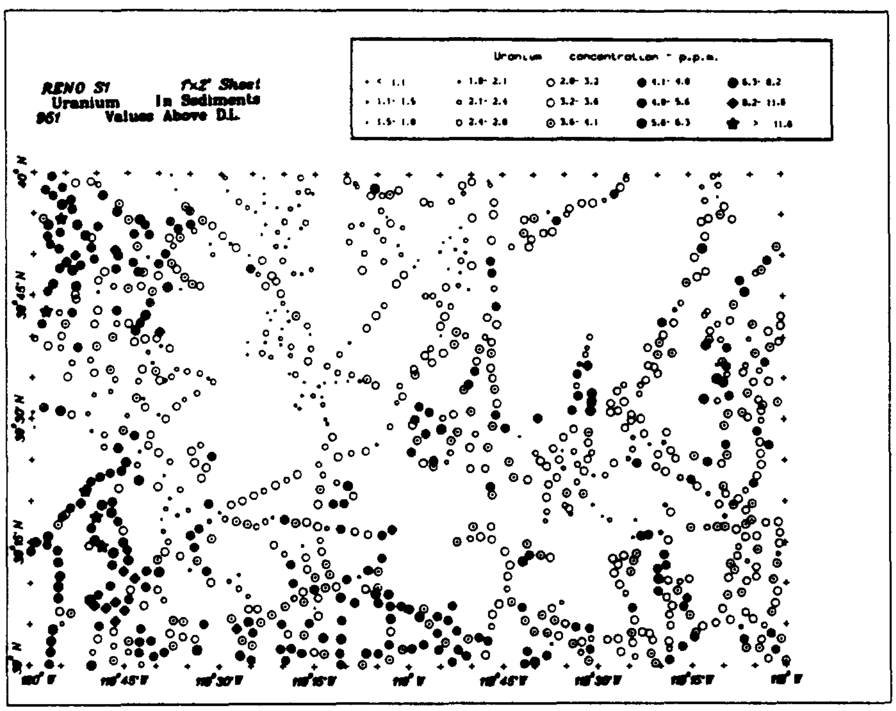


FIGURE 10. DISSPLA three-dimensional plot of hafnium in the Charlotte 1° x 2° quadrangle showing correlation between hafnium concentration and geology. Geologic contacts and unit names were hand drafted on figure. Figure from Price and Ferguson, 1978.

Computer graphics not only is an integral part of data reduction and interpretation, it also is a fundamental aid in the planning and forecasting of the NURE program at SRL. A case in point involves the question of how SRL sampling teams were to collect sediment samples in deserts. It had been the practice at SRL to analyze the fine fraction (-100 mesh) from each sediment sample. In deserts, however, fine particles can be carried tens of kilometers by the wind before deposition at a potential sampling site. It is evident that an elemental analysis of such transported sediment would not reflect the geology of the area from which the sample was obtained. It was decided, therefore, that both a fine and a ccarse sediment fraction would be analyzed from each sample obtained from an area in which airborne contamination could be deemed a problem. This course of action, however, doubled the analytical load for numerous western quadrangles; thus, the utility of analyzing two sediment fractions needed to be shown effective if the practice were to continue. Graphic representation of data from the Reno $1^{\circ} \times 2^{\circ}$ NTMS quadrangle (Figure 11) encouraged continuation of the two-fraction option. Inspection of the areal distribution plots (Figure 11) indicates that anomalous concentrations of uranium would have been missed in the northwestern (fine fraction) and southeastern (coarse fraction) parts of the quadrangle had not both the fine and coarse fractions been analyzed.





FIGURES 11a and 11b. Areal distribution symbol-plot maps of the Reno 1° x 2° quadrangle showing uranium concentrations in the coarse (S0) and fine (SØ) sediment fractions.

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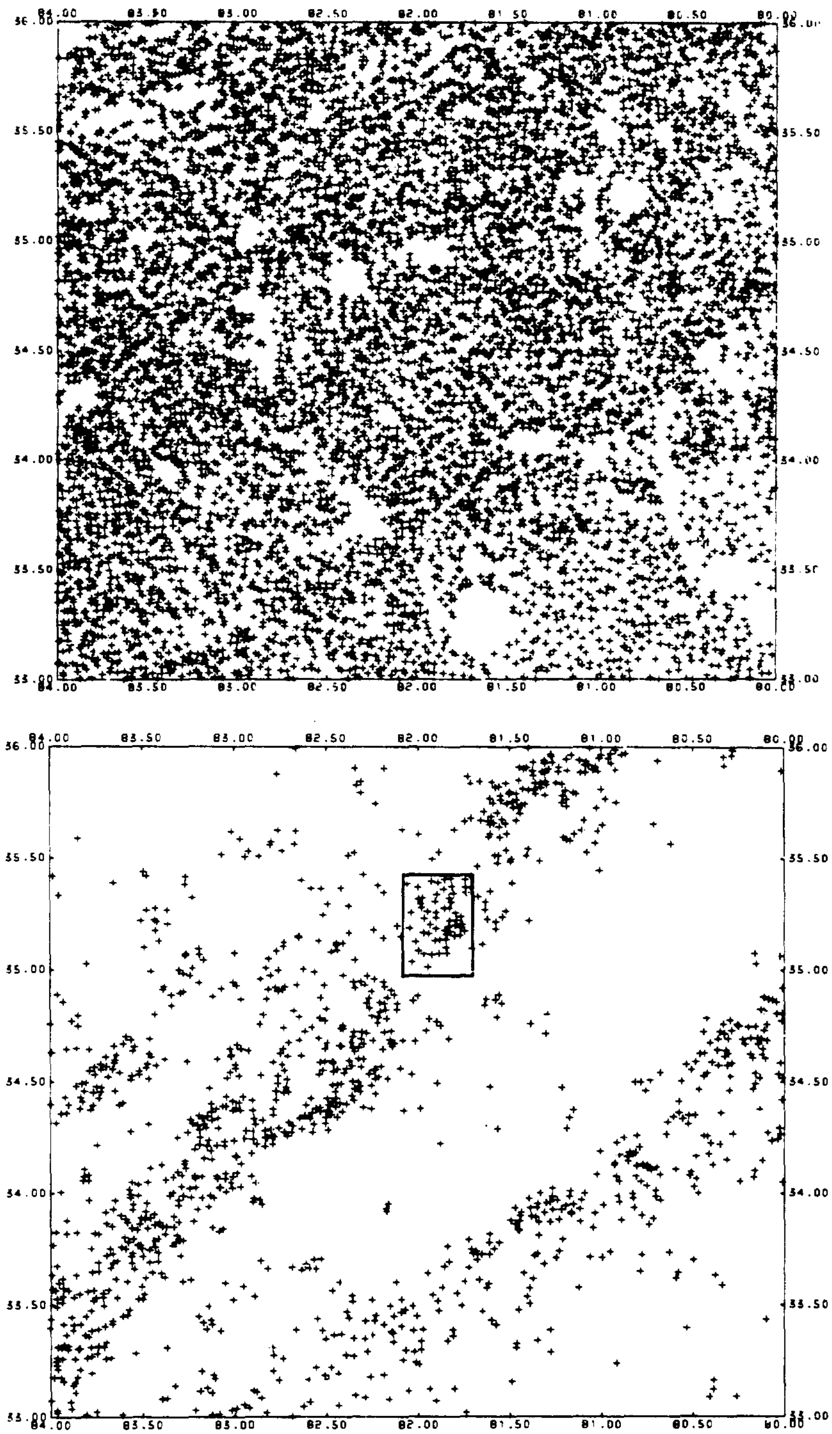
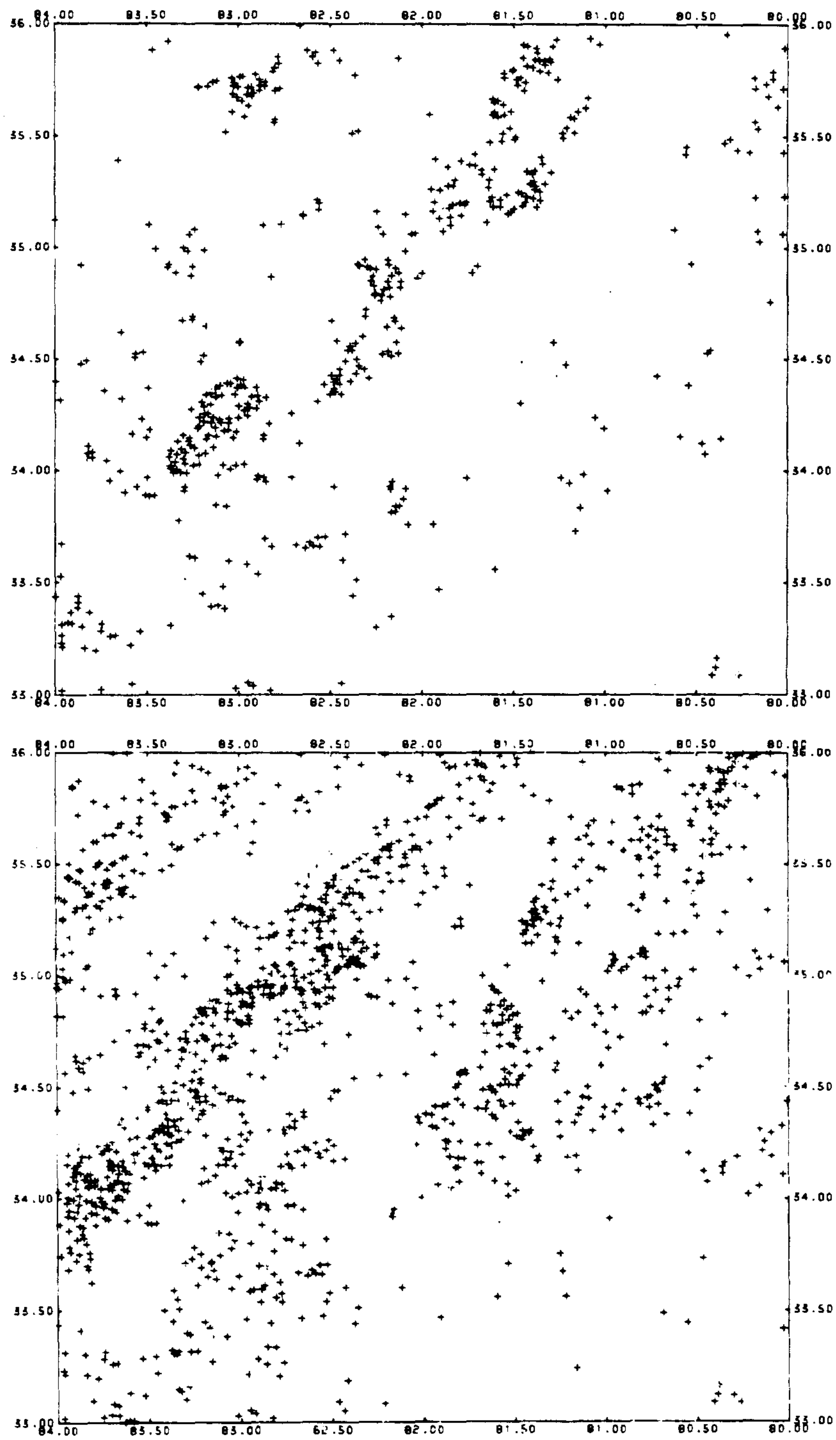
Plots, such as those in Figure 11, reflect the absolute concentration of an element in a sample and define anomalous areas. It can be demonstrated, however, that samples and areas having high concentrations of uranium, for example, are not necessarily the best economic prospects. Figure 12 is a SURFACE II posting of all sampling sites in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles from which a uranium value was obtained. It is the task of the NURE geologic staff at SRL to determine which of the samples represent economically extractable uranium reserves. A first step toward this end is represented by Figure 12b. A SAS routine was used to filter the uranium numbers so that only values of greater than 20 ppm were plotted. Figure 12b, therefore, depicts the location of samples with relatively high uranium contents. Uranium, however, in geologic terrain such as that represented by this six-quadrangle area often is incorporated in minerals from which the uranium cannot be extracted economically. Monazite [$(Ce,La,U,Th)PO_4$] and zircon [$(Zr,Hf,U)SiO_4$] are two such minerals which dominate the uranium-bearing mineralogy of most sediment samples from this area. It is a cogent argument, therefore, that the uranium contributed by these minerals to the uranium data set must be deleted in order that an analysis of economic deposits be valid.



FIGURES 12a and 12b. Figure 12a is a posting of sample sites in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles from which a uranium value was obtained. Figure 12b is a posting of only those sites with uranium values greater than 20 ppm.

To eliminate the effects of monazite and zircon, respectively, the U/Th and U/Hf ratios were calculated for each sample. In Figure 13a are displayed only those samples which have calculated U/Hf ratios greater than 0.6. Thus, the uranium in samples plotted in Figure 13a cannot be accounted for by zircon. Similarly, no samples with U/Th ratios less than 0.5 are plotted in Figure 13b. This figure depicts the position of samples in which the uranium likely cannot be attributed to monazite. To produce Figure 14, a compound filter was applied which combined the filters of Figures 13a and 13b. Therefore, the positions of samples in Figure 14 probably represent rocks most likely to contain economically extractable uranium. It is important to note that the samples within the hand-drawn rectangle on Figure 14 do not appear in Figure 12b. This indicates that although the samples of Figure 14 represent relatively favorable economic prospects, they are not anamolously enriched in uranium. Conversely, the samples within the hand-drafted rectangle in Figure 12b, in spite of having relatively high uranium concentrations, are not plotted in Figure 14. These samples, therefore, likely represent relatively poor prospects. It can be inferred from this example that the geology of an area must be integrated with elemental analyses if an effective prospecting tool is to be obtained. Also, without the aid of computer graphics, it is clear that regional analyses such as these discussed here would be exceedingly cumbersome, if not impossible, within realistic budgets and reasonable time limits.



FIGURES 13a and 13b. Figure 13a is a posting of sample sites in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles which have U/Hf values greater than 0.6. Figure 13b is a posting of U/Th values greater than 0.5 for the same area.

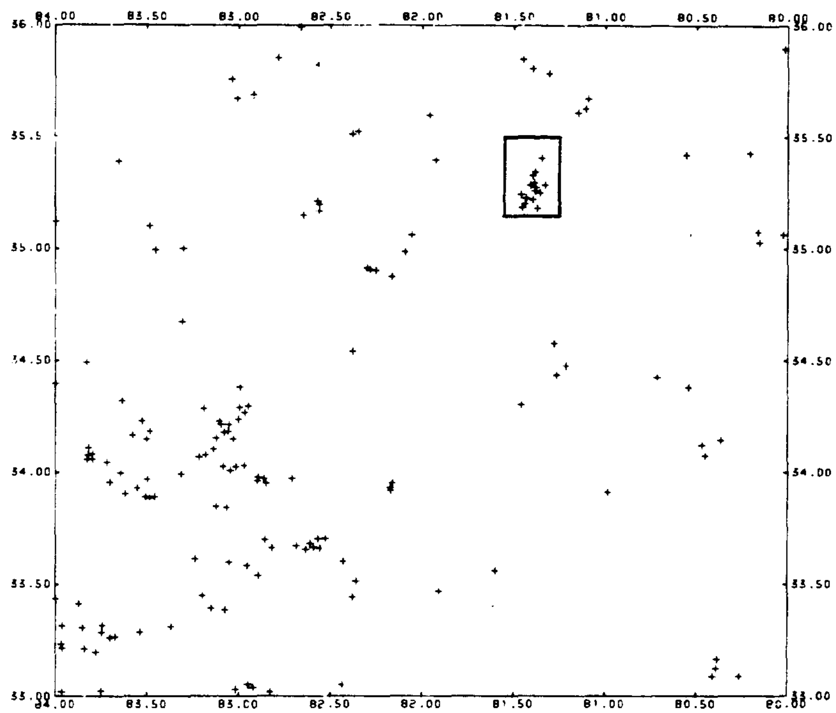


FIGURE 14. Posting of sample sites which have U/Hf values greater than 0.6 and U/Th values greater than 0.5 in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles.

CONCLUSION

It has been demonstrated by example that computer graphics is an essential tool for the geologic staff at SRL. Computer graphics not only allows more rapid execution of tasks which could be performed manually, but also presents scientists with new capabilities which would be exceedingly impractical to apply were it not for the application of computer graphics to a problem.

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FIGURE CAPTIONS

FIGURE 1. SRL area of responsibility.

FIGURE 2. SURFACE II contour map of log U/Hf in Portland 1° x 2° NTMS quadrangle. Eastern portion of map is Atlantic Ocean.

FIGURE 3. SURFACE II contour map of uranium in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles.

FIGURE 4. SURFACE II three-dimensional plot of uranium in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles.

FIGURE 5. Contour map of residual uranium values in central and western South Carolina.

FIGURE 6. Posting of sample sites from which calculated uranium residual values are greater than 0.15.

FIGURE 7. DSSPLA plot including an areal distribution symbol-plot map, a histogram, and a cumulative frequency plot of uranium values in the Albany 1° x 2° NTMS quadrangle.

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FIGURE 14. Posting of sample sites which have U/Hf values greater than 0.6 and U/Th values greater than 0.5 in the Knoxville, Charlotte, Greenville, Spartanburg, Athens, and Augusta 1° x 2° NTMS quadrangles.