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A User's Guide to SURFACE: An Interactive Program for
Creating Pictures and Movies of Three-Dimensional Surfaces

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December 15, 1976

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A User's Guide to SURFACE: An Interactive Program for
Creating Pictures and Movies of Three-Dimensional Surfaces*

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Abstract

In many cases, scientifically important problems cannot be well represented for visual interpretation in two dimensions. For example, in the case of potential energy surfaces, two-dimensional plots are often insufficient. Additionally, the available data in these problems tends to be rather sparse -- at least by computer graphics standards. SURFACE is a computer code designed to operate with Livermore Time Sharing System hardware and software. The program's purpose is to facilitate comprehensive analysis through the generation of three-dimensional figures from sparse data sets and the production of a 16 or 35 mm movie of the surface from a wide range of perspectives.

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Introduction

SURFACE was created with the following need in mind: given an experimental data set where each element of the data set is composed of three variables (i.e., pressure:temperature:volume,time:energy:population), each element can be considered to be a point in three-dimensional space (X, Y, Z). These "points" can be conveniently and meaningfully displayed as a plot of one variable against the other two, resulting in a surface (Figure 1).

For many experiments, however, the data collected may be rather sparse, and some manipulation must be done to "fill in" the unknown values in order to construct a smooth, continuous surface. Viewing two-dimensional displays of three-dimensional objects, some information is lost. To recover this information, it is usually necessary to view the object from many different perspectives in order to fully understand the significance of the available information. SURFACE was designed to fulfill these requirements.

Background

During the summer of 1976, a need arose within the Theoretical Atomic and Molecular Physics Group of the Laser Program to be able to transform calculated potential energy data into a meaningful graphical representation. Concurrent with this need had been the introduction and refinement of PLOTPK (UCID-30125), a graphics package allowing easier access to the Livermore time-sharing system's TV80-LIB subroutines. SURFACE was our subsequent answer to the physics problems that utilized the relevant commands of PLOTPK.

Using SURFACE, user-scaled (X, Y, Z) data is arranged on a 50 x 50 grid. This matrix is filled in by interpolation, and the full grid is "smoothed" to give a reasonable three-dimensional surface which is consistent with the original data. This surface is then displayed on a TMDS (CRT) monitor and can be rotated at will to provide a total perspective of the surface. If the picture is satisfactory, a movie showing rotation of the surface about its center can be created (16 mm or 35 mm), and the movie can be further processed by LLL's Technical Information Department to add color, titles, etc.

Access to SURFACE is gained through the following ELF command:

```
ELF RSL .049625:MOVIE:SURFACE
```

which will transfer the most current SURFACE controllee (assuming PHOTOSTORE is up). SURFACE executes PLOTPK,¹ which is a public file on the LTSS CDC7600 computers.

¹ SURFACE itself runs quite well at priorities of one or below. When PLOTPK is involved, it may be necessary to increase your priority in order to maintain adequate response times.

Further information on PLOTPK can be accessed through the PLOTPK manuals (UCID-30125, Parts I and II) or by contacting PLOTPK's author, Peter Keller. Questions or comments regarding SURFACE should be addressed to L. A. Cox, Jr.

Data Set Format

Data for SURFACE must be of the form (X, Y, Z) where X and Y are the coordinate locations of Z , the "height" of the surface at that location. SURFACE places the Z -component into a 50×50 matrix using X and Y as the subscripts. This requires X and Y to be integers from 1 to 50, which means that some data preprocessing must be done by the user to appropriately scale the data. As the final matrix is sent to PLOTPK with the FORTRAN format (F10.4), it is suggested that the Z data be scaled to fall within the range $(-10,000, 1,000,000)$. The data (X, Y, Z) should be constructed to conform to the right-hand coordinate system, with Z as the "height" of the surface above the X, Y plane.

Suggested Procedure

The following sequence of instructions has been found to be the most useful and optimal way to produce a smooth three-dimensional plot:

1. Create data set (X, Y, Z) as disk file (see FILE).
2. FILE command - initially enters data.
3. INTERP command - interpolate to fill in matrix.
4. SMOOTH command - first smoothing operation.
5. NO-OUT command - turns off output of statistical messages.
6. CYCLE command - sequential FILE/SMOOTH/EDIT commands.
7. PLOT command - display plot on TMDS.
8. Return to item 6 for further smoothing as needed.
9. MOVIE command - produces surface rotation movie if desired.

The individual commands are more elaborately detailed in the command language section.

Upon initial execution of SURFACE, the following message is printed to the TTY:

```
ENTER X, Y COORD. (INTEGER 1 TO 50), VALUE (FLOATING PT.)  
ENTER 'END' TO TERMINATE INPUT.  
OPTIONS ARE:  CYCLE EDIT FLIP FILE PLOT INTERP STOP SMOOTH NO-OUT  
              MOVIE END  
OK.
```

All commands to SURFACE must be entered after an OK., which is printed upon successful completion of each command. All commands and options must be blank delimited, one command per line.

Surface Command Language

TTY Data Entry

After any OK., a data point (X, Y, Z) may be entered by typing X and Y as blank delimited integers from 1 to 50, followed on the same line by Z as a blank delimited floating point number with ten or fewer

total digits (including decimal point). This will place Z in the data matrix at location (X, Y), initializing that location OR REPLACING THE PREVIOUS VALUE. Successful placement of Z will result in an OK. response.

This entry method is useful for replacing "strange" data points but should be used only for temporary debugging. The CYCLE command requires that all data points be in a disk data file, so any points entered by TTY will have little effect on the final surface if CYCLE is used.

FILE

The FILE command will normally be the first command entered after the first OK. The command line is

FILE filename

where filename is the name of the LTSS (ASCII) disk file containing the (X, Y, Z) data. The disk file must have the following format:

X_1	Y_1	Z_1
X_2	Y_2	Z_2
.	.	.
.	.	.
.	.	.
X_n	Y_n	Z_n
END		

where X and Y are integers (1 to 50) and Z is a floating-point number with nine or fewer digits. The program will respond with statistics about the data unless the NO-OUT command has been executed.

INTERP

The INTERP command normally follows a FILE or the end of a sequence of TTY data entries. The command line is

"INTERP"

INTERP fills in the unfilled coordinates of the 50 x 50 matrix with interpolated values derived from the input data to produce a rough surface. A call to SMOOTH after INTERP will flatten out the rough areas in the surface.

INTERP must be called once before SMOOTH is executed for reasonable surfaces to result.

SMOOTH

The command SMOOTH changes all values in the 50 x 50 matrix in an attempt to make the surface more continuous and smooth. The command line is

"SMOOTH"

The present procedure for smoothing is a weighted, six-nearest-neighbor average for the new value of each point. SMOOTH may be executed sequentially as many times as desired, but occasional calls to FILE will help maintain data consistency.

NO-OUT

It will be observed by the user of SURFACE that a variety of messages are sent to the terminal by an executing SURFACE, from the OK prompt to statistics resulting from the current command. The NO-OUT command can be used to suppress output of these messages or restore the output feature if called a second time. The messages normally sent to the TTY are sent to the SURFACE LOG file named "SLOG." The command line is

"NO-OUT"

Users may find some of the information contained in the log file of interest. Several X-Y plots (in line printer/RJET format) are included, one of which is a plot of the relative positions of the input points from which the interpolation is made. Since "dayfile" like information is also included, some files can grow quite large, so some caution is advised when printing the log file on slower devices such as Versatec printers.

CYCLE

The CYCLE command causes a user-specified number of calls to FILE/SMOOTH/EDIT for maximum consistency of surface with original data and for a more pleasing visual presentation. The command line,

"CYCLE"

will cause the prompt

ENTER NUMBER OF CYCLES, FILENAME,

for which the user should type the integer number of cycles and the data file name, i.e.,

20 DATAFILE

If NO-OUT has not been called, the messages resulting from each execution of FILE and SMOOTH and EDIT are printed. For any number of CYCLES greater than one, this becomes lengthy and tedious.

WARNING! CYCLE can use significant amounts of CPU time. We advise that you try a CYCLE/PLOT sequence with approximately five cycles each time and a priority below 1.0 to avoid unnecessary charges.

PLOT

The command

"PLOT"

will cause SURFACE to take three steps:

1. SURFACE will request the number of the TMDS monitor you wish to use:

TV ???

to which you should respond with the one to three digit number.

SURFACE will then request your box number and identification:

BOX # ?? (ANN) ID ?? (MAX. 10 CHARS.).

Reply with your computer box number (i.e., Y04), and a ten character identifier to be attached to any PLOTPK output (see UCID-30125, specifically the BOX10 command).

2. Any old file named PLPKOUT will be destroyed and a new one created. Into this new file will be written the data matrix and some PLOTPK commands (MACROS) described below.

3. PLOTPK will be executed.

The operating system will respond

PLOTPK STARTED BY +SURF

and after some delay (depending on system load, your priority, etc.) your surface will appear on the TMDS. A period (.) prompt from PLOTPK will be typed when PLOTPK is ready to receive commands. At this point, PLOTPK has complete control, and any of the commands in Peter Keller's manual are usable.

About the plot: the initial perspective can be thought of as though the viewer were in the (+X, +Y, -Z) octant of the left-handed coordinate system,

with the origin $(0, Y_{\text{MIN}}, 0)$ as the lower left corner of the cube displayed (see Figure 2). The X-axis increases left-to-right, the Z-axis increases front-of-cube to rear-of-cube, and the Y-axis increases bottom-to-top. From SURFACE to PLOTPK, a coordinate transformation has occurred. The data operated on by SURFACE came from the right-handed coordinated system (X, Y, Z) with Z vertical. PLOTPK assumes that the vertical axis is the Y axis. To the user, what all this means is that what was previously labeled (X, Y, Z) is labeled in PLOTPK as (X, Z, Y) . We hope this will not cause too much confusion.

Four special commands have been included by SURFACE for users who are unfamiliar with PLOTPK. These commands let you view the surface from different perspectives in order to better grasp the available information.

VFRONT - returns the view to the $(+X, +Y, -Z)$ perspective seen in the first plot.

VLEFT - the viewer appears to be on the left side of the surface relative to the VFRONT view.

VRIGHT - viewed from the right side.

VREAR - backside view.

The view commands can be executed as many times, in any order desired, after each . prompt. A convenient PLOTPK command to use between view commands is RJ, which outputs the view to any LTSS RJET with a Versatec printer.

After viewing the plot and executing any PLOTPK commands desired, return to SURFACE by typing END. This terminates PLOTPK, outputs any PLOTPK files to the appropriate device, and returns control to SURFACE. SURFACE will prompt

WHAT NEXT?

The user has two options here:

1. Type END to terminate SURFACE.
2. Carriage RETURN returns to the command input mode and prompts with OK.

Plot may be called after any OK to view any stage of the surface development. It may be necessary to increase your priority to get reasonable response times as PLOTPK is a rather large code.

MOVIE

Once the surface has taken an acceptable form, it is often desirable to be able to see the plot from a variety of perspectives sequentially to get a better grasp of the surface characteristics. This is conveniently done by making a movie displaying the rotation of the surface.

The command

"MOVIE"

goes through the same three steps as PLOT, with the first step expanded to include user selection of the movie's characteristics. The questions MOVIE asks and their required responses are:

1. BOX # ? (ANN) ID ? (10 CHAR. MAX.) - Your box number (e.g., Z48) and an appropriate identifier (e.g., ENERGY PLOT) are required by the people at Computations so that the correct movie gets to the appropriate people.
2. ENTER YES TO KEEP FILES, ELSE RETURN - PLOTPK allows the option of creating the movie and sending it to the operating system for processing (hit RETURN) or for more sophisticated users, keeping the movie files on disk (type YES).
3. ENTER YES TO SHOW MOVIE ON TMDS, ELSE RETURN - You can see the movie as it is being made on a local TMDS monitor by entering

YES here, then giving the monitor number when asked for. If you do not wish to view it, hit RETURN.

WARNING! Entering YES will not only tie up the monitor for an extended period of time, it will also burn an extravagant amount of both real and computer time.

4. 16 OR 35 MILLIMETER FILM? FOR 35 WITHOUT HARD-COPY, ENTER 35M -
Three movie output options are available: 16 mm film, 35 mm film, or 35 mm film with xerox hard-copy of EACH FRAME. Quickly, black-and-white movies are normally made by entering 16 mm. Movies to be further processed by TID (John Blunden), such as colorizing, titling, etc., would be 35M. Enter 35 only for movies with few degrees of rotation, or if you desire several pounds of xerox hard-copy.
5. AXES LABELS? (10 CHAR. MAX. EACH) X Z Y - As explained before, PLOTPK uses left-handed coordinates, the X-axis increasing front-back, and the Y-axis bottom-top. These correspond to the data axes (X, Y, Z). You must enter all three labels (blank delimited) or none at all (see Figure 2).
6. FREEZE TIME FOR INITIAL VIEW (INTEGER SECONDS)? - The initial perspective for the movie is the same as the initial perspective from the PLOT command. This view will be "frozen," with the axes labels just entered, for the number of seconds entered here, based on 24 frames per second. The initial freeze is to give the viewers time to recognize the axes and for your introductory remarks. Twelve to fifteen seconds seems to be adequate. Default is twelve if nothing is entered.

7. HIDDEN LINES REMOVED? 0 = NONE REMOVE, 1 = SURFACE REMOVED, 2 = SURFACE AND BOX - PLOTPK has a built-in, hidden-line algorithm for deleting hidden surfaces and box lines. 0 usually creates a strange plot (Figure 3); 1 may leave box lines around (Figure 4); 2 seems to be best, removing all hidden lines not related to the desired view (Figure 5). Default is 0.
8. PLOT BOX? 0 = NONE, 1 = BOX, 2 = WITH SIDEBARS, 3 = WITH LABELS - The box around the surface is a perspective convenience that is often best left out. 0 eliminates box and sidebars (Figure 6), 1 leaves box in but sidebars out (Figure 7), 2 adds sidebars (Figure 8), 3 is default, with box sidebars, and labels on the Y axis (Figure 9). The Y axis labels are numeric limits on the range of Y and are usually indecipherable anyway.
9. TOTAL MINUTES ROTATION TIME? (REAL #) - The total time the movie will take up is the sum of the answers to items 6 and 9. The answer to 9 (default 1.0 minutes) determines increment of rotation angle between successive frames when coupled with 10.
10. TOTAL DEGREES OF ROTATION? (REAL #) - Beginning with the initial perspective at (+X, +Y, -Z), the movie will display the figure rotating counterclockwise about its center for the requested number of degrees (270.0 default).
11. BLUNDENIZED? YES OR RETURN - John Blunden of TID was of enormous help in formulating this program. As a potential saving of computer time, it is recommended that a Blunden factor of two or three be used (answer YES, will prompt for number). What this does is increase the angle of rotation between succes-

sive frames, which decreases the total number of frames created. The film should be done as 35 mm, then taken to John who will duplicate each frame by the Blunden factor specified here and reduce the 35 to 16. This process will maintain desired time and rotation while reducing computer generation time. Any factor above three will cause the movie to appear with jerky, uneven motion. Default factor is two if YES is entered and no number is entered for the prompt.

After you have answered all of the above questions, put your priority at one or below and go have a cup of coffee, unless you requested viewing on TMDS. The process of creating 2500 vectors for each frame, with 24 frames per second of movie (non-Blundenized), takes some time. The movie will automatically be sent for processing unless you requested to keep it, in which case your total disk area used increases dramatically. Upon completion, the message

MOVIE COMPLETED PLOTPK DONE

is printed and control returned to SURFACE, as at the end of PLOT.

MOVIE INTERRUPT: If for some reason you desire to break off the movie before completion, type STOP. This will cause PLOTPK to interrupt, returning to a prompt. If you do not want the frames currently on disk to be sent for processing, type ABORT. To return to SURFACE, type END.

EDIT

The EDIT command replaces values in the 50 x 50 matrix such that all points are within the range of the data read in by FILE ($\pm 10\%$) or set equal to a constant used by SURFACE to label uninitialized points. The purpose of EDIT is to keep the matrix mathematically self-consistent

with the original data and delete any points whose interpolated value is probably unjustified by the input data. The command line is

"EDIT"

FLIP

As previously noted, a transformation from (X, Y, Z) to (X, Z, Y) is effected in going from SURFACE to PLOTPK, the transformation being merely in labels. It occasionally happens that a user creates a data set in such a manner that what he thought was (X, Y, Z) is treated by SURFACE as (Y, X, Z), which results in the plot being rotated 90 degrees to (Y, Z, X). Should this occur, END SURFACE, restart it, and enter FLIP as the first command. This will cause any data points entered to be treated as (Y, X, Z). The program responds

WHAT?

and retypes the preliminary information on available options. Each execution of FLIP causes a reversal of (X, Y, Z) to (Y, X, Z) to (X, Y, Z), etc.

STOP

The

"STOP"

command will terminate SURFACE, leaving behind file SLOG, which contains output information useful for debugging, and file PLPKOUT, if PLOT or MOVIE was ever called.

END

The

"END"

command should be used to terminate data entry by TTY if only TTY is

used. It will attempt to do an interpolation. If the data is too sparse for SURFACE to use, the message

NOT ENOUGH DATA TO INTERPOLATE - TRY LINEAR FIT
will be printed and SURFACE will end.

Special Applications

A user with sufficient expertise in using both SURFACE and PLOTPK can create quite complex plots, even with multiple surfaces per plot (Figure 10). These are particularly striking when each surface is done in a different color. For further details, see P. Keller or S. Levine of the Computations Graphics Group, or John Blunden of TID.

Our special thanks for assistance and patience go to John Blunden, Peter Keller, Steve Levine, Caroline Hunt, Wendy Grady, and Dr. C. F. Bender.

FIGURE 1

FIGURE 2

FIGURE 3

FIGURE 4

FIGURE 5

FIGURE 6

FIGURE 7

FIGURE 8

FIGURE 9

FIGURE 10

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