Computer Software Reviews

SCI-GRAF. Version 1.10E. Microcomputer Systems Consultants: 32 West Anapamu, Suite 190, Santa Barbara, CA 93101. List price $99.95.

SCI-GRAF is a scientific graphics program designed to produce high-quality graphs in color or black and white on dot-matrix printers. The copy reviewed was fully compatible with IBM computers and could be used with a variety of different printers. MS-DOS or PC-DOS version 2.0 or later and a minimum of 256K of RAM are required, but to utilize all of the available options 640K of memory is recommended. According to the documentation provided, a Hercules card option exists, but it was not mentioned during the installation procedure and various difficulties were encountered when this card was present: no screen image was produced, and the program would "hang" rather than return to the main menu.

SCI-GRAF is very similar to Scientific Plotter obtained from Interactive Microware, Inc. (P.O. Box 139, State College, PA 16804) in all respects, but the output on a printer is somewhat better, and it is possible to do graphs in color with SCI-GRAF. Both of the programs permit data to be plotted on rectangular, semilog, and log–log grids both with and without error bars. Scientific Plotter permits bar graphs and pie charts. It should be noted that SCI-GRAF is restricted to dot-matrix printers and cannot be adapted to plotters.

The review copy of SCI-GRAF contained the program FONTEDIT, available at $39.95, which is used to create custom characters. This option permits the introduction of Greek letters and other symbols in labels on the graphs. By using this option it was a trivial matter to create a benzene ring character, for example. The print-out is proportionally spaced, so care must be taken to prevent overwriting parts of the custom characters. The printer used in this evaluation was a TI 855 with a custom character module. FONTEDIT is practically identical with the TI-LOAD program obtained from SoftStat, SFS (2651 Delcane Drive, Columbus, OH 43220) for loading custom characters into the TI font module. FONTEDIT is hardware independent.

SCI-FRAF produces excellent graphs exactly as described in the manual. It is exceptionally easy to use, and it can be used in conjunction with data files obtained from other devices provided that data can be cast in the form of a series of numbers. In the present instance, kinetic data from a fast transient digitizer can be test plotted as first and second order with ease. Initial interaction will require 1–2 h in order to become familiar with all of the options present in the software. Significantly more time is required if custom characters are to be created with FONTEDIT. The inner workings of the program are not made available. One has no idea how the graphs are generated, nor can one assess the precision of the placement of a point plotted on the graph. The software is not intuitive from the screen. The manual is helpful and must be used at all times. This is especially true in FONTEDIT since the function keys are defined *only* in the manual. In an effort to accelerate the user's progress, the program advances at each key stroke and does not allow errors to be fixed without exiting to the main menu and beginning again. The software does not lend itself to modification, but examples are given for using programs in C, Pascal, and Basic to generate data. Modules are available from the vendor at $250 which permit linking high-level graphics functions to programs written in C.

The graphs produced by SCI-GRAF are of excellent quality, and they are readily obtained. While they are most useful in qualitative applications such as graphs for slides, posters, and other presentations, the graphs could also be used in dissertations and reports. It is unlikely that the graphs produced by dot-matrix printers will be useful for publication, especially if they are in color. In all other circumstances, both academic and industrial chemists could use SCI-GRAF to great advantage.

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GAUSS. Version 1.49B. Aptech Systems Inc.: P. O. Box 6487, Kent, WA. List price $200.00 for the language, $50.00 per each of three additional module packages.

GAUSS is a complete programming language integrated with an operating environment and some powerful analysis packages. Its purpose is to give users the ability to perform "mainframe" scale computations on an IBM PC/XT/AT, IBM System/2, or compatibles. The advantages of GAUSS stem from an ability to efficiently manipulate arrays, enabling one to write programs which handle large amounts of data in a clear and concise fashion. Gauss itself is written in optimized assembly language making full use of the math coprocessor (8087 or 80287 chip,

19 digit precision) so its programs also run fast and are numerically accurate. Provided in the modules are tools for the treatment of linear as well as nonlinear systems of equations, to output publication quality graphics, do statistics, signal processing, and handle a variety of other problems. Be forewarned that GAUSS, as any computer language, demands the user take the time to learn its syntax and command set and is therefore not software that can be fully mastered in any brief period.

The GAUSS program sets up an environment from which the user switches between a command mode and an editing mode. There are no menus in either mode, nor any on-line help to speak of, so it is not particularly user friendly. From the command mode you can run compiled programs or write then interactively run small (in terms of size, not ability) programs. For example generating a 2048 point vector of exponentially decaying cosine waves, taking the Fourier transform, then plotting the results to the screen and a dot matrix printer took only six lines of code and ran almost immediately. GAUSS could be used strictly as a very capable math scratchpad in this manner, but it is limited to the code that fills the screen. The edit mode is designed for writing longer programs allowing each procedure to contain hundreds of lines (64K limit). A single function key will automatically save, compile, and run, reporting any discovered error with a message and line number. There are some useful debugging features in the language for when these error messages become too cryptic. Both modes have full screen editing capabilities that are easy to use but nothing extraordinary, and any ASCII editor can be used to write programs as the language contains no special symbols.

The GAUSS language is algebraic and even inexperienced programmers will have no problems picking up the basics, although those familiar with C will feel most at home. Matrix operations are carried out from a single line of code with implicit dimensioning. For example, without any prior reference to x the statement

$$x = y/z$$

will compute x by division if y and z are both scalars, divide every element of y by z to produce matrix x if y is a matrix and z a scalar, or attempt a matrix solution of the system $y = zx$ if both y and z are matrices. The standard functions work on an array of any size within an 8190 element limit and the language features various file handling commands, screen and printer I/O commands, logic statements, statistical functions, and an impressive list of matrix operators. Along with inverse, pseudoinverse, Schur Decomposition, eigensystem analysis, and the like are commands to reshape, concatonate, even deal with individual rows and columns. In short, it seems nothing has been left out of the basic language.

Associated with GAUSS are 12 modules that contain various applications programs. The first comes with the language, while the others are sold separately in three packages as modules 2–6, 7–11, and 12. Aptech includes the source codes so that users can tailor them for specific needs as desired, but I found them of more immediate value in providing programming insight. Module 1 contains some nice procedures for 2-D plotting such as displaying multiple graphs with each containing multiple functions simultaneously. There are serious limitations here in supporting only CGA graphics and producing hardcopy via screen dumping. Modules 2–6 cover file handling, statistics, regression, statistical analysis, and systems of linear equations. Modules 7–11 contain routines for treating nonlinear equations and doing signal processing. This includes nonlinear least-squares, solving simultaneous equations, estimation, and optimization programs. Real and complex FFT's, inverse FFT's, convolutions, etc., are featured in the signal processing module. Module 12 is an extensive graphics package, more sophisticated than module 1. It handles both 2D and 3D plotting with log, semilog, polar, contour, and surface plots. Output can be sent to most of the standard dot matrix printers, laser printers, plotters, and Hercules, CGA, and EGA cards are supported. The plot data are stored in a high-resolution (4190×3120), Tektronix format so that hardcopy quality is dictated more by the device than the software.

The manual for GAUSS is well written, but I found an immediate need to add some dividers and shuffle around a few sections. Documentation for the modules comes on their disks and needs to be printed out. The commands and procedures are nicely detailed along with examples of their usage, but there are some basic elements absent. For instance, there are several commands that manipulate complex arrays but

nothing on how to input or define one, unnecessarily adding to the manual-searching/experimentation aspects of programming in a new language. Installation did not exactly follow the written procedure, apparently confusing module additions with the basic language installation, but nothing anyone with a knowledge of DOS will have much trouble with. Included in the manual are five tutorial lessons that do a good job in introducing beginners to GAUSS' divers capabilities. There are some errors in the text, not only here but in the modules as well, mostly of a typographical nature such as neglecting to define one of the variables in a 3D plot. Worse is that it is not always clear when certain procedures or default parameters must be loaded prior to attempting to follow the examples. Most of these problems are cosmetic, especially in comparison to the normal difficulties encountered when using a new programming language and in attempting to perform tasks formerly unattainable on a PC.

GAUSS lets you have full access to DOS and any other programs on disk without leaving the environment, so you can change directories, copy files, even use it to build up batch programs. It is also possible to interface with routines written in Assembler, or C and FORTRAN providing one has a compatible compiler. It even comes with a de-installation program for removing all associated sub-directories from a hard disk and the escape key works.

GAUSS is not copy protected and can be run on a system with two DS/DD drives but is best installed on a hard disk. It requires DOS 2.1 or higher, a math coprocessor, and at least 320K RAM. A CGA graphics card is needed for use of module 1, 512K and any of the standard graphics cards for module 12. Aptech is constantly revising the

program(s) and entitles owners to their updates. There is also a GAUSS newsletter, subscriptions are $12.00 per year. It might be difficult to run this program with less than 640K since the program inherently challenges its users to push around large amounts of data, though there are commands in the language for dealing with freeing up previously used memory. Unfortunately, 640K is also the maximum memory utilized regardless of how much is on the system.

The closest competitor of GAUSS is probably PC-Matlab by Math Works, and both have very similar capabilities. Matlab is more expensive, is copy-protected, and does not currently have the graphics output capabilities of Module 12, but it does have a better user interface with good on-line help and parallel versions that run on mainframes as well as the Macintosh. Asyst by MacMillan Software (see *J. Am. Chem. Soc.* **1987**, *109*, 3178) is also more expensive and copy protected, but it more powerful. It has interfacing capabilities for data acquisition and can handle 65 000 elements with up to 16 dimensions per array as compared to GAUSS's limit of 8190 elements and 2 dimensions. The GAUSS language is somewhat easier to learn, but this is subject to the individiual programmer's preference.

In summary, GAUSS is a good programming package of interest to anyone desiring to do serious computation on a personal computer. It is versatile, powerful, fast, accurate, and relatively affordable. These features far outweigh the inconvenience of a scant user interface. If your calculations can stay within GAUSS' array size and memory limitations, it will allow you to push your PC to the best of it's number crunching abilities.

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Book Reviews *

Handbook of Polycyclic Aromatic Hydrocarbons. Volume 2: Emission Sources and Recent Progress in Analytical Chemistry. Edited by Alf Bjørseth and Thomas Ramdahl. Marcel Dekker, Inc.: New York. 1985. 416 pp. $95.00 (U.S. and Canada); $114.00 (all other countries). ISBN 0-8247-7442-6

This book updates and expands upon the very useful first volume. It consists of eleven chapters, by widely recognized experts, covering most of the current areas of activity in this field. The extensive chapter by S. A. Wise on HPLC updates his chapter in Volume 1. It provides extensive data sets, comparisons of HPLC and GC/MS data on U.S. National Bureau of Standards Standard Reference Materials, and Figure 7, which reproduces the HPLC chromatogram of eleven pentacyclic $C_{22}H_{14}$, is a delight to those of us who have hitched our fortunes to this technique. The Chapter by K. D. Bartle updates the GC chapter in Volume 1. It emphasizes advances in open tubular column GC and expands upon higher molecular weight polycyclic aromatic hydrocarbons (PAH) and derivatives such as nitro-PAH which are commanding increasing attention. The introductory chapter by Bjorseth and Ramdahl on Sources and Emissions of PAH is valuable not only as a literature compendium but also because of the balanced and introspective nature of the review which points up inconsistencies and uncertainties in reporting emissions, for example, in the selection of specific PAH and the definition of total PAH. Bjørseth has also co-authored a later chapter wth G. Becher concerning Determination of Occupational Exposure to PAH by Analysis of Body Fluids. This is an important current area and the authors nicely provide discussion of the pathways PAH follow in living animals and humans. One wishes that there was also discussion of the recoveries of the metabolites in human urine using their technique. Three chapters on PAH emissions from sources [Coal-Fired Plants (K. Warman), Biomass Combustion (T. Ramdahl), and Automobiles (U.R. Stenberg)] follow the first chapter. The eighth chapter on Analysis of 6-Nitrobenzo(*a*)pyrene in Mammalian Cells and Microsomes by HPLC is a departure in style in that it is more specific, using this compound as an archetype for other nitro-PAH. We now know that 1-nitropyrene, 2-nitropyrene, and 2-nitrofluoranthene are considered to be more significant atmospheric mutagens. Chapter 9, by D. W. Later, concerns Nitrogen-Containing Polycyclic Aromatic Compounds in Coal-Derived Materials and concerns azaaromatics as well as amino- and cyano-PAH rather than nitro-PAH. The following chapter by Van Cauwenberghe concerns Atmospheric Reactions of PAH and is well organized and summarized including differences in particulate- and gas-phase reactivities. This Reviewer

wishes that a bit more was done to explain the relationship between molecular properties of PAH (besides Free Valence) and reactivity; there is interesting discussion in the 1980/81 literature of the relation of Diels–Alder reactivity of PAH with the gap between the first two ionization potentials of the PAH. The final chapter by Karcher, Reference Materials for the Analysis of Polycyclic Aromatic Compounds, advertises the PAH standards available from the Commission of the European Communities and provides useful discussion on preparation, purification, and purity criteria.

Although this book was published in 1985, it is still very current and will be a useful addition to institutional libraries and the bookshelves of research practitioners. One wishes that there was also coverage of "biologically driven" analysis of pollutants (e.g., by Ames assay) which has indicated the importance of polar derivatives, analysis of indoor PAH, and analysis of PAH metabolite/DNA adducts, but perhaps these will appear in a future volume.

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Food Chemistry. By H. D. Belitz and W. Grosch. Translation from the second German edition by D. Hadziyev, University of Alberta, Edmonton, Canada. Springer Verlag: New York. 1987. 774 pp. $79.50.

Few textbooks on Food Chemistry treat the subject as exhaustively as the above-named one. The table of contents is complete enough to give one a thorough idea of what is discussed in the book. Equally detailed is the index. An "Appendix of Selected References to the Literature of Food Chemistry and Related Fields" will be of help to students, especially those entering the field.

Organization of the text follows, more or less, the traditional format. The contents may be divided into sections as follows: Section I, chemical components of foods (water, amino acids, peptides, proteins, enzymes, lipids, carbohydrates, aroma substances—a complete chapter is devoted to each of the above-named topics); in section 2, Chapters 10–18 deal, in consecutive order, with major food products (milk and dairy products, eggs, meat, fish and other aquatic animals used as food, fats and oils, cereals and cereal products, vegetables and their products, fruits and their products); section 3 is composed of four chapters—Chapter 19 discusses sugars, sugar alcohols and honey while alcoholic beverages are treated in Chapter 20, and coffee, tea and cocoa are dealt with in Chapter 21 and spices, salt and vinegar in Chapter 22.

Although Food Science and Food Chemistry are undergoing rapid and dynamic developments, the book is quite up to date, granting time lapses for translation and publication. The very brief preface presents some useful definitions of foods, Food Chemistry, etc., and stresses the im-

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*Unsigned book reviews are by the Book Review Editor.