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TITLE: VAXMATH: A MATHEMATICAL SOFTWARE LIBRARY FOR THE VAX

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VAXMATH: A MATHEMATICAL SOFTWARE LIBRARY FOR THE VAX

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ABSTRACT

VAXMATH is a large collection of mathematical software for the VAX, based in large part upon the SLATEC Library. Routines in the library represent the state-of-the-art in numerical mathematics and have been thoroughly tested. The library is characterized by the inclusion of many easy-to-use routines, the use of a standard error handler, and machine readable documentation. Specific information on how to obtain the software is available.

INTRODUCTION

Over the last few years, the VAX has proved to be a very popular computer with scientists at the Los Alamos National Laboratory. As these machines are used more and more for scientific computations, fundamental changes have been required in the mathematical subprogram libraries. In this paper we will not only discuss the development of VAXMATH, but will trace the acquisition of the current collection of mathematical software available at Los Alamos. We will discuss the specific impact of shorter word length machines on our computing environment and describe some of the difficulties encountered in actually building a mathematical subprogram library for use on the VAX. Information will be given on how to obtain the software, and the available documentation programs for the library will be discussed.

VAXMATH

VAXMATH is a portable mathematical software library currently containing approximately 800 routines written in Fortran. Although its usage is intended for VAX/VMS, it will run with minor alterations on other operating systems.
The current version of the library has routines in the following areas:

Area	Origin
Special Functions	FNLIB
Basic Linear Algebra	BLAS
Linear Equations	LINPACK
Eigenvalues/Eigenvectors	EISPACK
Nonlinear Equations	MINPACK
Quadrature	QUADPACK
Initial Value Problems	DEPAC
Poisson's Equation	FISHPACK
Interpolation and Approximation	

Efforts continue to increase the number of routines in all areas of mathematical computation.

History

For years, a mathematical subprogram library has been built for each worker computer in the Central Computing Facility (CCF) at Los Alamos. Each library was provided as a binary public file, so that each individual user was freed from the task of compiling these basic mathematical utilities. By late 1979 the number of VAXes and VAX usage had increased to the point that the Los Alamos VAX Local Users Group recommended that a similar mathematical library be made available on the VAX. At that time the source was being collected for the SLATEC Common Mathematical Library, so naturally it was used as the foundation for VAXMATH.

SLATEC

SLATEC (Sandia, Los Alamos, Air Force Weapons Laboratory Technical Exchange Committee) was formed in 1974 by representatives of the computing groups of Sandia National Laboratories, Albuquerque; Los Alamos National Laboratory; and the Air Force Weapons Laboratory.

SLATEC was organized to foster the exchange of technical information among its members. To accomplish this purpose, subcommittees with specific charters were established. One of the first of these was the Common Mathematical Library Subcommittee, which in 1977 adopted a proposal to develop a common mathematical library.

The original three members of SLATEC have been joined by Sandia National Laboratories, Livermore; Lawrence Livermore National Laboratory; and National Magnetic Fusion Energy Computer Center. In addition, Union Carbide Corporation (Oak Ridge) and the National Bureau of Standards are members of the Math Library Subcommittee.

The SLATEC Common Mathematical Library was to provide a set of mathematical subroutines, written in Fortran, to aid in scientific computing at the participating laboratories. Goals for the library included portability, good numerical technology, robustness, good programming style, online documentation, and careful testing. When development of the library started, there were several free, high-quality software packages available. A number of these were made a part of the library. When this software did not conform to the user interface standards that had been established by the subcommittee, easy-to-use drivers were added rather than the original codes being modified. The library has routines in the areas listed previously. That list shows the origin of some of the routines. In some computing environments, all of the Ansi 77 mathematical intrinsic functions (SQRT, SIN, COS) are not vender supplied. The SLATEC library also contains a file of these routines written in Fortran.

In 1981 a preliminary version of the library was distributed to all SLATEC sites, and in April 1982, the first official version of the library was sent to member sites and to the National Energy Software Center (NESC) for further distribution. For more information on both SLATEC and the SLATEC Common Mathematical Library, see References (1) and (2).

IMPACT AND INSTALLATION

A major activity of many scientists at Los Alamos is the mathematical modeling of physical processes. For this reason the Central Computing Facility has developed around a core of supercomputers, the workhorse today being the Cray-1s. Originally the mathematical libraries, including the SLATEC Common Mathematical Library, were designed for use on these large supercomputers, generally characterized by long word length (60 bits or more). As this computing capacity was augmented by distributed processors, mainly VAX family machines, it became necessary to make some changes in library philosophy. At the same time, the VAX has gained popularity among other Department of Energy laboratories. This fact influenced the continuing development of the SLATEC Common Mathematical Library.

Impact of the VAX on Mathematical Library Development

Use of the VAX for scientific computing presented the Mathematical Library Subcommittee with a problem. It was decided that routines should be available that gave the same accuracy on these machines as computations done on supercomputers. Because the VAX has a 32-bit word, double precision counterparts of all single precision routines were required. By 1980 contributors to the SLATEC Common Mathematical Library were asked to supply both single and double precision versions of the routines submitted. Of the almost 800 routines in VAXMATH, approximately 170 are double precision, and we anticipate that more will be added.

All of the routines in VAXMATH have quick-check programs that provide adequate, but not exhaustive, tests. Many of these were originally written for use with the SLATEC library and failed when first run on the VAX. This failure was almost always due to error constants used for comparison in the test codes by asking for 10 to 12 digits of accuracy. This shortcoming in the quick checks was overcome by using significance tests relative to round-off error. In many cases this took the form of error constants like

(round-off error)**0.6.

This kind of check also benefited testing on other machines and significantly improved the quality of the SLATEC library.

Installation and Maintenance

In preparing the library, most things went smoothly. However, in some routines long error messages are printed (through the error handling subroutines XERROR or XERRWV), which require Hollerith strings to be continued on another line. These statements presented a problem because the VMS Fortran compiler will not count any trailing blanks through column 72 unless they are preserved by a text editor. Unfortunately, the text editor used at that time did throw away trailing blanks. To overcome this problem, the Hollerith string must be shifted so that a non-blank character is in column 72 or the blanks must be padded.

Another problem occurred while the library was actually being tested on the VAX. Any integer variable used to dimension a variable length array must be positive at run time or VMS aborts the routine. Several quick checks and user-callable routines were found that passed a nonpositive integer as an array length to a subordinate routine. These bugs were not discovered earlier because other operating systems at the Laboratory do not do this run-time check.

Originally most of the VAXes were purchased as standalone computers located at remote sites around the Laboratory. It soon became evident that there were advantages to being connected to the Central Computing Facility (CCF). This realization resulted in the development of XNET, sitting on top of DECnet and connecting these VAX distributed processors to the main computing facility. This connection gave users access to the worker computers, file storage, printing and graphics facilities, and other services. In December 1981, the Computing Division extended the change control procedure to software provided by the Division for all VAX distributed processors. When new or modified software is available, its access on the CCF Common File System is restricted to the VAX system managers, and the managers are responsible for installing the software on their systems. VAXMATH is also maintained in this way. Distribution of VAXMATH among standalone VAXes is done by tape.

DOCUMENTATION AND DISTRIBUTION

Although not part of VAXMATH, a documentation program is available for the library and is distributed with the SLATEC source. In the development of the SLATEC library, the Mathematical Library Subcommittee decided unanimously to provide machine-readable documentation. To do this, standards for the prologues and the classification system were adopted. A documentation program was written, keying on the precise information in these standards. Most subprograms in the library source had suitable prologues, and those that did not were expanded. Specific comment statements were added to all SLATEC sources in compliance with the following standard that was adopted for the prologues for the user callable subprograms.

```
C***BEGIN PROLOGUE
C***DATE WRITTEN
C***REVISION DATE
C***CATEGORY NUMBER
```

```
C***KEYWORDS
C***AUTHOR
C***PURPOSE
C***DESCRIPTION
C***REFERENCES
C***ROUTINES CALLED
C***END PROLOGUE
```

We will further explain three of these categories. Under C***CATEGORY NUMBER are one or more categories in the Bolstad classification system (3). Under C***PURPOSE are one to six lines of information on what the subprogram should do and the types of problem solving for which it was designed. Under C***DESCRIPTION are the program abstract, methods used, argument descriptions, dimension information, consultants, and other pertinent information.

Other Documentation Programs

Because of the prologue and classification standards, others have written documentation programs keying on characteristics in these standards. Tom Jefferson of Sandia National Laboratories, Livermore, has written an interactive online documentation program, MATHDOC (4). He wrote this program specifically for the VAX, using the VAX library facility. One of our co-authors, Jeff Chow, is currently working on a portable interactive online documentation program using a direct-access approach. Robert Boland, another co-author, is working on a program to generate hardcopy documentation from the online prologues. All these documentation programs use the standards set forth for the prologues and the classification system.

Distribution

VAXMATH is not distributed separately because it was built almost entirely from the SLATEC Common Mathematical Library. In April 1982, the official version of the SLATEC library was sent to the National Energy Software Center for external distribution. A copy of the SLATEC tape (NESC No. 820) is available on a subscription basis from NESC, 9700 Cass Avenue, Argonne, Illinois 60439.

CONCLUSION

At Los Alamos, most large-scale computations will still be done on the CCF supercomputers, but we foresee more and more preprocessing activities being done on distributed processors. Thus, we must provide mathematical routines that run well on distributed processors and, with minimal changes, also run on the worker computers. We must also provide routines with the same accuracy as those available in the CCF. The current VAXMATH collection is a valuable first step in this direction.

REFERENCES

1. Buzbee, B. L., "The SLATEC Common Math Library," Sources and Development of Mathematical Software, W. Cowell, Ed., Prentice-Hall Series in Computational Mathematics (to appear).

2. Vandevender, W. H., and K. H. Haskell, "The SLATEC Mathematical Subroutine Library," ACM SIGNUM NEWSLETTER, September 1982, pp. 16-21.

3. Bolstad, J., "A Proposed Classification Scheme for Computer Program Libraries," SIGNUM NEWSLETTER, Vol. 10, No. 2-3, November 1975, pp. 32-29.

4. Jefferson, T. H., "MATHDOC and SLATEC, A User's Guide," Sandia National Laboratories, Livermore, Report SAND82-8767, June 1982.