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The PORT Mathematical Library has been installed on an IBM PC-XT equipped with 640 Kbytes of RAM, 8087 coprocessor, DOS 2.0 operating system and MS Version 3.20 FORTRAN compiler. Necessary editing of the original files to conform with this configuration is described, along with the techniques for loading on a machine with limited memory compared to mainframe machines. Installation of the storage stack and error handling routines has been tested and found completely successful. Those of the approximately 1400 mathematical routines which have been tested and/or used have proven totally satisfactory. The author will be glad to supply the files, preprocessed for use on the PC, to anyone who is interested; machines other than IBM which are DOS 2.0 compatible should be suitable for use in this regard. The availability of such a mathematical library should increase the value of a desktop stand-alone machine to chemists and physicists for such uses as data handling and model calculations among others.

Remarks

Approved By: <i>L. A. Farrow</i> L. A. Farrow	<i>M. J. Bowden</i> M. J. Bowden	<i>J. M. Rowell</i> J. M. Rowell	Date July 24, 1984
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## ABSTRACT

The PORT Mathematical Library has been installed on an IBM PC-XT equipped with 640 Kbytes of RAM, 8087 coprocessor, DOS 2.0 operating system and MS Version 3.20 FORTRAN compiler. Necessary editing of the original files to conform with this configuration is described, along with the techniques for loading on a machine with limited memory compared to mainframe machines. Installation of the storage stack and error handling routines has been tested and found completely successful. Those of the approximately 1400 mathematical routines which have been tested and/or used have proven totally satisfactory. The author will be glad to supply the files, preprocessed for use on the PC, to anyone who is interested; machines other than IBM which are DOS 2.0 compatible should be suitable for use in this regard. The availability of such a mathematical library should increase the value of a desktop stand-alone machine to chemists and physicists for such uses as data handling and model calculations among others.

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IBM-PC-XT  
Project Number: R0500

DATE: July 24, 1984  
FROM: Leonilda A. Farrow  
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TM-ARH-000051

TECHNICAL MEMORANDUM

**1. Introduction**

The personal computer has already attained memory size and computation speed sufficient to perform many of the types of calculations useful to chemists and physicists.<sup>1</sup> This ability would be greatly enhanced if a mathematical library such as the Bell Laboratories PORT package, with its roughly 1400 programs, were adapted for PC use. Such an adaptation has been made successfully for the IBM PC-XT with surprisingly little difficulty. Since many machines are compatible with the PC-DOS operating system, application need not be restricted to the PC-XT, although the availability of the 10 Megabyte hard disk for storage is convenient.

Documentation on the contents and capability of the PORT library has been splendidly done elsewhere.<sup>2</sup> Hence this paper will be confined to discussing the modifications, mostly minor, which had to be made for conversion to the PC. The changes were occasioned almost entirely by the expected need for machine constant conversion and by some differences between the mainframe (Honeywell and Cray) FORTRAN compilers and the PC FORTRAN compiler, which has proven to be generally robust. Loading problems which arise because of the limited RAM size of the PC (640 kilobytes maximum) will also be considered.

**2. Configuration of the PC-XT**

The essential hardware consisted of one system unit, containing a 10 Megabyte hard disk drive and a floppy disk drive, a monochrome screen, and an asynchronous communication port connected to a Hayes 1200 Smartmodem. RAM memory was extended to 640 kilobytes, which is the maximum amount that can be addressed with the PC's 16 bit word size. Originally, only 256 Kbytes were available; this amount was found to be a severe constraint on the size of program which the compiler could handle. Finally, the 8087 floating point chip was added to speed up all subsequent number crunching.

Software was based on IBM PCDOS 2.0. The FORTRAN compiler was Microsoft Version 3.20, which takes advantage of the 8087. In order to obtain the PORT files, use was made of the terminal emulator program SIMTERM<sup>3</sup> which facilitates communication between the PC and the VAX UNIX system. PCDOS comes equipped with a line editor, but this was discarded in favor of the IBM Personal (Screen) Editor, which greatly

facilitated the extensive stand-alone editing which is described in a subsequent section.

It may be of interest to note briefly the results of some timing tests<sup>4</sup> conducted with the above hardware and software configuration. Two tests were performed, the first consisting of a dot product loop, the second a row operation loop, each with 10,000 operations. The IBM PC was found to be about 5 times slower than the VAX 11/750, but about 60 times faster than an AT&T 3B2 without hardware floating point. As yet, no comparison is available for the AT&T PC 6300.

### 3. UNIX Preprocessing of the PORT Files

The PORT Library is arranged in chapters<sup>2</sup>, covering the following general subjects:

- Framework
- Utilities
- Approximations
- Differential Equations
- Fast Fourier Transforms
- Linear Programming
- Optimization
- Quadrature
- Roots
- Sparse Matrix
- Special Functions

(For details, the reader should consult reference 2.) Each subject, or chapter, listed above was originally available on the Honeywell on a single file. These files were sent, one at a time, to a VAX using the `hget` command. This transfer was made to facilitate editing the files so that Hollerith strings were enclosed in single quotes, as required by the PC FORTRAN COMPILER, rather than being preceded by `nH`, where `n` is the number of characters in the string, as was done in the original files.

Since the files are large, ranging in size from approximately 7000 to 20,000 lines, a program was written to seek out and perform the essential format changes.<sup>5</sup> The program was unable to operate on the files without first splitting them into more manageable size. The UNIX command `split` with an option size of 300 lines was found convenient. Regrettably, it was also necessary to erase the identifying columns 73-80 on each line before applying the editing program. This left unnecessary trailing blanks at the end of each line which were eliminated to cut down on the number of characters to be downloaded. A program was written<sup>5</sup> which performed all of these operations at one time on all of the split files, which might number in excess of 50 for a large chapter.

After this preprocessing, the files were downloaded onto the PC hard disk using SIMTERM.<sup>3</sup> The downloading was done using the small split files to cut one's losses in case of irretrievable interruption in the transfer process; this seemed to be more likely when the UNIX machine was very busy. Weekend downloading of large files was always successful in the writer's experience; during the regular work week such attempts were nearly always unsuccessful.

### 4. Editing and Testing the PORT Files on the PC

After the procedures outlined above were completed, all remaining work was done on the PC standing alone. The **Frame** and **Utility** chapters were naturally the first to be run through the FORTRAN compiler, since they contain those programs which set up the storage stack<sup>2</sup> and do the error handling.<sup>2</sup> They also contain the routines for returning the real, floating-point, and integer constants which must be set for the IBM-PC with the

8087.<sup>5</sup> All other PORT Library programs must be run in conjunction with these background routines.

In order to optimize speed and decrease size of object and execute files, it is necessary to add two Microsoft FORTRAN metacommands, which are **Sstorage:2** and **Snofloatcalls**. The first of these appears just once in a source file as the very first statement, and forces all integers to be 2 bytes instead of 4. Those integers which must be 4 bytes will remain unaffected by this command if declared **integer\*4** rather than **integer**. Declaration for some of the machine constants had to be altered in this manner. The **Snofloatcalls** command was inserted at the beginning of each subroutine to insure that all floating point operations were performed with direct calls to the 8087 rather than with time-consuming interrupts.

The first run through the FORTRAN compiler failed because of the presence of format array statements, which are allowed in full FORTRAN 77 but not in the subset implemented by the MS version 3.20 compiler. For example, as originally written, a format statement with 12 characters would be placed in a dimensioned array with 12 entries. A simple fix for this problem is as follows. On the PC, suppose that a format array is declared

```
character*1 fmt(12).
```

(On the mainframe machines, the declaration is **integer** instead of **character\*1**.) It is only necessary to create another array

```
character*12 ffmt
```

and add the statement

```
equivalence (fmt(1),ffmt).
```

All read and write statements using **fmt** must be changed to **ffmt**. These changes take a certain amount of editing; however they are needed only in the **Frame** and **Utility** chapters. The screen editor mentioned above was found to be very helpful in performing this work.

It should be noted that, because of the format problem encountered in this work as just discussed, a special editing program has been written<sup>5</sup> and applied to the PORT files. Thus the version to be released as PORT3 will not need the special editing described above.

Once the **Framework** and **Utility** chapters were successfully compiled, a series of standard tests<sup>2</sup> was run to check the PORT linguistic hypotheses, the installation of the machine constants, the automatic error handling, and the stack allocator. Standard messages were returned if all ran correctly. It was found that the messages were somewhat garbled, with three out of four letters missing. The problem was traced to the necessity of changing **IMACH(6)**, the number of characters per word, from 4 to 1 in the function **IIMACH(D)**. This represents the difference between declaring Hollerith characters as **integer** (4 to a word) on the mainframe machines and declaring them as **character\*1** on the PC. With this change, the expected messages appeared for all tests, indicating successful installation of the **Frame** and **Utility** chapters.

Since this work was initiated, Microsoft has issued Version 3.20.1, which has the ability to handle Hollerith strings preceded by nH for writing, but not reading. IBM has also issued a compiler, which appears to be a copy of MS 3.20.1 except for its inability to recognize and/or handle complex numbers.

## 5. Loading

On a mainframe machine, all of the PORT library may be loaded and subroutines called at will. However, on the PC, with its maximum 640 Kbytes of memory, such a procedure is clearly impractical. The user will therefore have to load subroutines as needed. Fortunately, all programs have been thoroughly cross-indexed<sup>2</sup> as to which subroutines call and are called by others. The library has also been arranged so that needed subroutines are almost always in the same chapter. The **Framework** (object) file should always be loaded. If memory is at a premium, it is not necessary to load all of the utility chapter, which contains some specialized programs such as fast sorts. The cross-indexing<sup>2</sup> mentioned above gives the specific utility programs needed for a given case.

In order to facilitate collection of just the required subroutines, the UNIX command `fsplit` has been transferred to the PC. `fsplit` splits up the large chapter files into smaller files, each one of which contains just one function or subroutine, and names the file with the function or subroutine name appended by `.f`. For example, subroutine `setr` will appear as a separate file called `setr.f`. One can then concatenate the necessary separate files using the DOS command `COPY`.

As a final note, during the linking stage the `8087.lib` should be the only math library loaded in order to optimize for speed and to take advantage of the `Snofloatcalls` command discussed in an earlier section.

The need to consult the cross index can be eliminated by first splitting each chapter file into its constituent functions and subroutines using `fsplit` and then compiling each of the resulting files separately. The object files so obtained can be organized into a library (using software such as the program `POLYLIBRARIAN`<sup>6</sup>) which is kept on floppy disks. The linker can then ask for the disk and select the necessary subroutines as needed, much as it now selects from the standard FORTRAN library supplied by the compiler software. Such a procedure is clearly to be preferred, and is in process of being implemented.

In addition to the files containing the PORT subroutines, there is another file containing all of the examples printed in the PORT User's Manual. Since there are approximately 1400 subroutines available, it was clearly not practical to test all of them. However, those that have been tested and used in actual problems have been found to work perfectly, thus encouraging continued extensive use of this library on the PC.

## 6. Conclusion

Installing the PORT library on the IBM PC-XT has proved to be comparatively simple. For those who are interested, the writer will be glad to supply the source files already treated for smooth handling by the PC FORTRAN compiler. The availability of such an excellent and extensive mathematical Library should extend greatly the value of a desktop stand-alone machine to chemists and physicists for such necessary tasks as data analysis and model calculations. This value will surely increase as Megabyte RAM memory in such machines becomes available, along with software support to take advantage of the greater memory size.

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L. A. Farrow

Atts.

References 1-6



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