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Recent Advances in Microprocessors for Analytical Chemistry

G. Horlick

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Recent advances in microprocessors for analytical chemistry

By G. Horlick
Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

The nature of scientific and electronic instrumentation is currently undergoing revolutionary change as a result of the development of microprocessors. These remarkable devices have permitted the development of a new class of intelligent instruments whose capabilities far exceed those previously thought possible. Among the features now provided in analytical instrumentation as a result of built-in microprocessors are automated analyses, the local availability of very large amounts of mass storage, a powerful data-processing capability at each instrument, self-testing and calibration, and information management software. The nature and consequences of these developments are discussed in this paper. In addition, the 'consumer market' computers are beginning to make a significant impact on analytical instrumentation and laboratories. The capabilities and role seen for such systems are outlined.

Introduction

While microprocessors have become standard components in scientific instrumentation over the last few years, the true impact of these subsystems is really only now beginning to be felt. The first implementations were just simple substitutions: at the high end as a replacement for a minicomputer and at the low end as a replacement for hard-wired conventional logic chips. However, the role of microprocessors in instrumentation is now rapidly progressing beyond these first somewhat pedestrian applications to where the complete nature of a measurement system or an instrumental technique is fundamentally altered as a result of the capabilities of current microprocessor subsystems. The word subsystem here is meant to be taken in the broadest sense in that not only is the basic computing hardware important but it is the impact of the complete data acquisition – data processing hardware and software package that must be assessed. These sophisticated systems are now available primarily as a result of the driving force of the demand from consumers, small businesses and hobby enthusiasts. We, as scientists, shall soon completely satisfy the vast majority of our computing needs by using products designed primarily for the above market and in fact benefit significantly from the development of hardware and software that would not have been developed solely for scientific use. Microprocessor systems are now available that are supported by access to vast amounts (several megabytes) of local memory on Winchester discs and sophisticated local computing power by means of array processors, have access to large local and networked scientific and personal data bases, implement input–output communication by voice, have sophisticated application software in the area of financial planning, data-base management and word processing, are portable and have excellent low-cost laboratory data-acquisition hardware and data-processing software packages. Taken together and placing all these capabilities in a bench-top instrument or on a scientist's desk fundamentally alters the role of computing in the laboratory. One sees stand-alone instruments capable of accessing extremely large data bases stored perhaps on video discs, performing sophiticated pattern-recognition algorithms with array processors, supervising short-term and long-term (archival) storage and retrieval of laboratory data and literature references by means of data-base management programs, automatically writing reports with word processing software, automatically diagnosing system failures over phone line connections to a manufacturer's headquarters and all the while conversing with the operator by voice input–output. While this complete scenario has not yet been implemented in one instrument or office, all the subcomponents exist and such systems are perhaps not far away.

In the next section examples will be presented of preliminary approaches to second-generation microprocessor-based instruments; the capabilities of a popular consumer computer will be summarized and some future directions will be outlined.

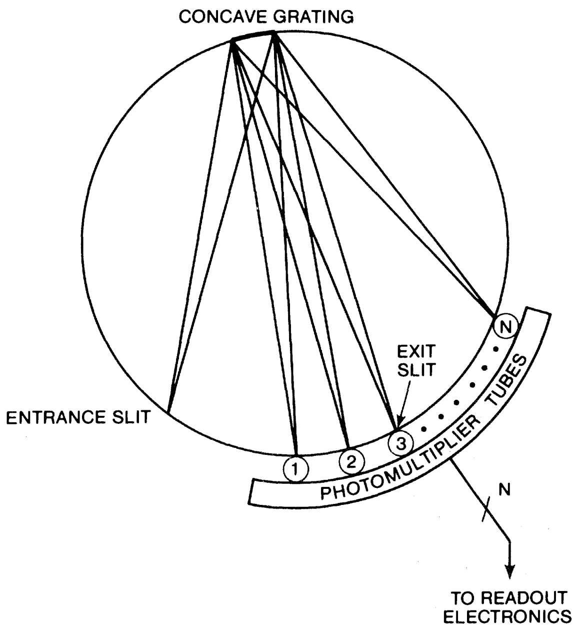

FIGURE 1. Polychromator optical arrangement.

MICROPROCESSOR APPLICATIONS

The nature of simple microprocessors and their basic role and capabilities with reference to analytical chemistry have recently been the subject of a special issue of *Talanta*. In that issue a series of articles provide an introduction to microprocessors (Horlick 1981), a discussion of interfacing fundamentals (Codding 1981) and a summary of the laboratory data-aquisition capabilities of several microcomputers (Salin *et al.* 1981). In addition, several examples of laboratory applications of microprocessors are presented, including read-out systems for photomultipliers (Blades & Horlick 1981), a system for acquisition of kinetic data (Gampp 1981), a reaction ratemeter (Ryan & Ingle 1981) and a simple data logger (Belchamber & Horlick 1981). Generally these applications fall into the first generation of microprocessor implementations as mentioned above. Two applications will now be outlined that begin to bridge the gap between these first-generation approaches and a more integrated approach.

Microcomputer-based polychromator

The polychromator, or, as it is often called, the direct-reading spectrometer, is widely used in emission spectrochemical analysis coupled to spark sources or inductively coupled plasmas. A simple optical arrangement for a polychromator is shown in figure 1 and a general block

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diagram of a typical measurement system in figure 2. In many ways the basic approach to the measurement system has not changed since its conception in the 1940s, except for the addition of electronic analogue–digital conversion and a minicomputer. Current signals from the photomultipliers are simultaneously integrated with analogue integrators; integrated values are then sequentially multiplexed to a single analogue–digital converter and then to the minicomputer. The integrated value may be read once at the end of an analytical run or may be read several times during a run (shorting the capacitor each time) with subsequent summation of the multiple readings to form a complete integrated value. This second approach requires considerable computer action during the analytical run.

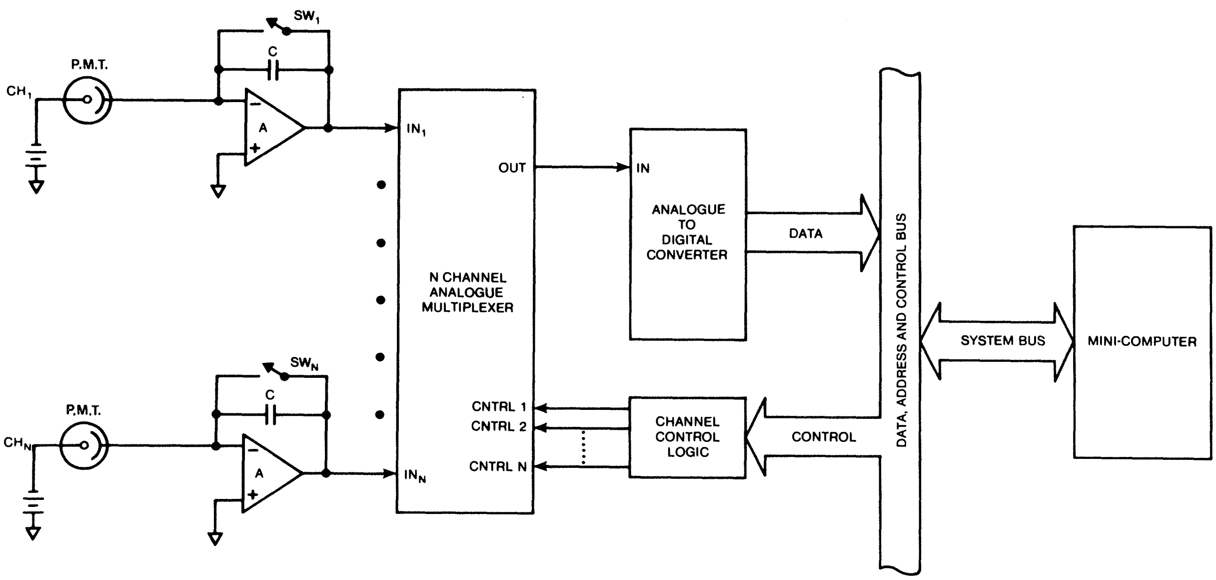

FIGURE 2. Block diagram of a traditional polychromator readout system.

An alternative configuration for a polychromator measurement system is shown in figure 3. This approach is based on a more complete utilization of modern microprocessor bus architecture, programmable support chips, inexpensive data domain-conversion chips and inexpensive single-board microcomputers. This system is an extension of the single channel design of Blades & Horlick (1981). Analogue integration is replaced by domain conversion of the current to a frequency and integration–digitization by a single-chip software programmable counter, the Intel 8253. The counters (a $12 integrated circuit) are completely programmable and can be addressed, configured, cleared, preset and read by simple software commands. This provides significant flexibility in overall system control since each channel is on the computer bus, in contrast to the more traditional system shown in figure 2.

The microcomputer used for this application was the inexpensive (*ca.* $500) microprocessor known as the Rockwell AIM-65. The hardware features of the AIM-65 and the memory allocation are listed in tables 1 and 2. This is a very powerful system that combines onto a single board almost all the features that one could want for basic data logging and instrument control: hard copy, high-level language, full keyboard, ease of interfacing. In addition many support products are available to enhance the capability of the AIM-65. It can be highly recommended for low-level applications.

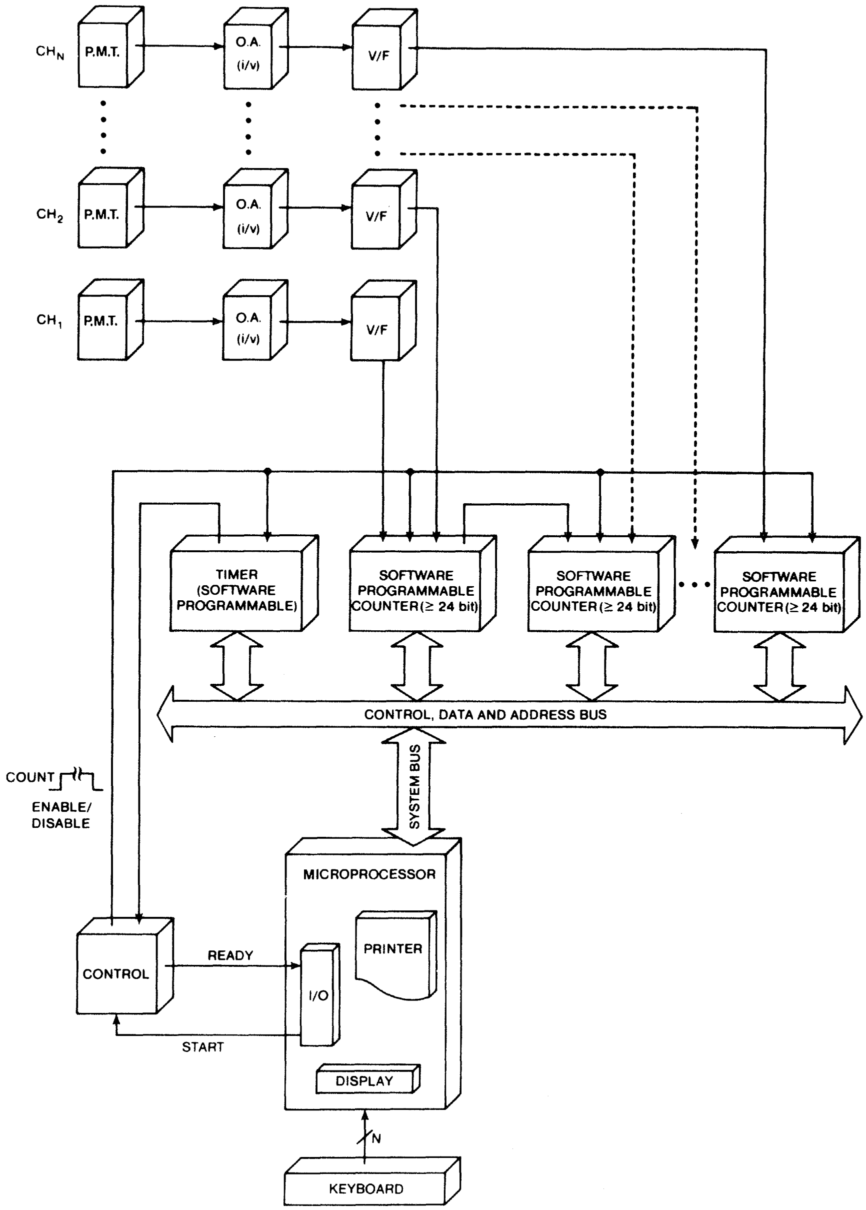

FIGURE 3. Block diagram of a microprocessor-based polychromator readout system.

TABLE 1. AIM-65 HARDWARE

20 column thermal printer	1 TTY interface
20 column display (16 segments)	1 6522 VIA
typewriter keyboard	1 expansion port
2 cassette interfaces	

TABLE 2. AIM-65 MEMORY

4kbyte read–write memory		8kbyte BASIC–read-only memory
8kbyte monitor	or	8kbyte FORTH–read-only memory
4kbyte assembler–read-only memory		

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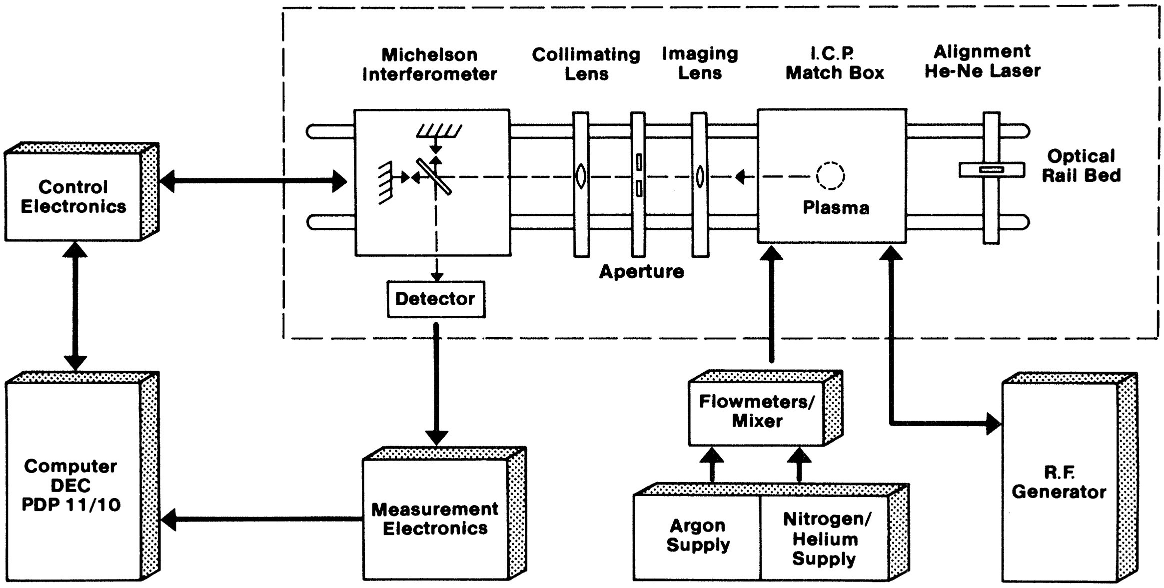

FIGURE 4. Block diagram of an i.c.p.–F.t. spectrometer system.

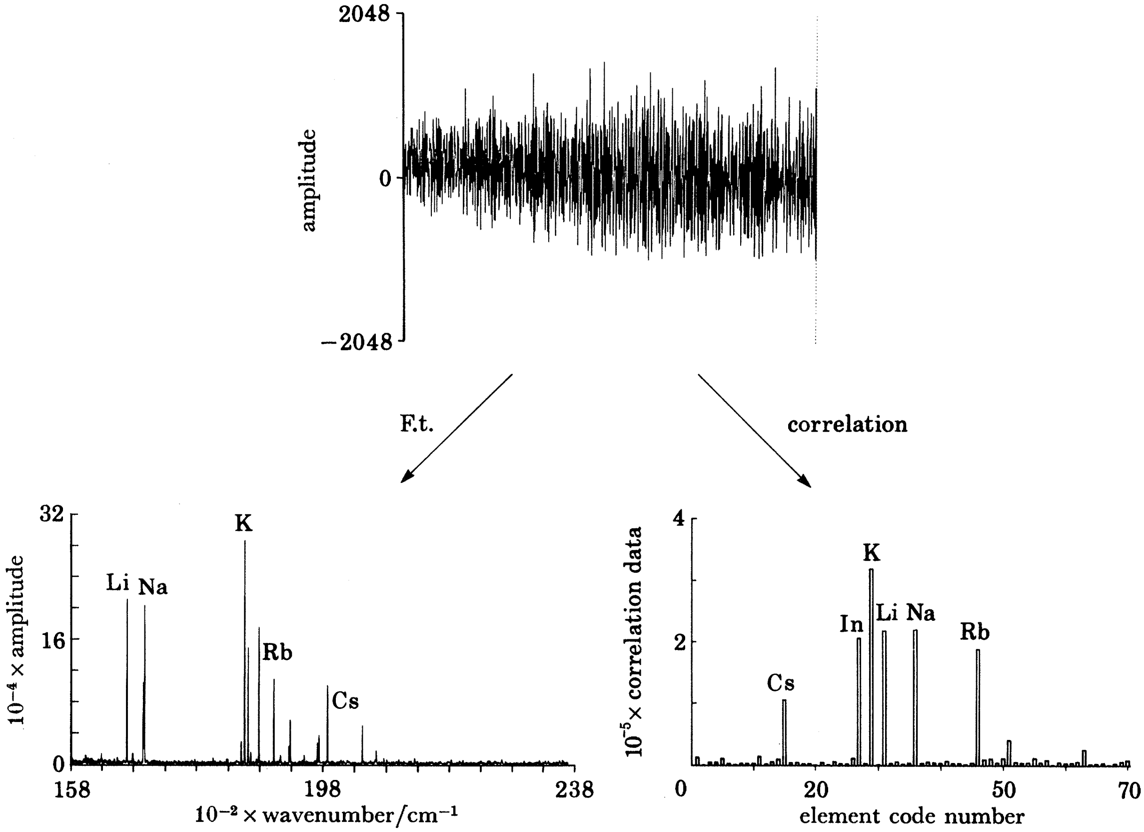

FIGURE 5. Comparison of F.t. and correlation data processing of an interferogram.

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Microcomputer processor for Fourier transform spectroscopy

Over the last few years we have been developing a Fourier transform (F.t.) spectrometer for application to atomic emission spectrochemical analysis (Yuen & Horlick 1978; Horlick *et al.* 1982). A block diagram of the current system as coupled to an inductively coupled plasma (i.c.p.) is shown in figure 4. Normally, the output signal from an F.t. spectrometer, an interferogram,

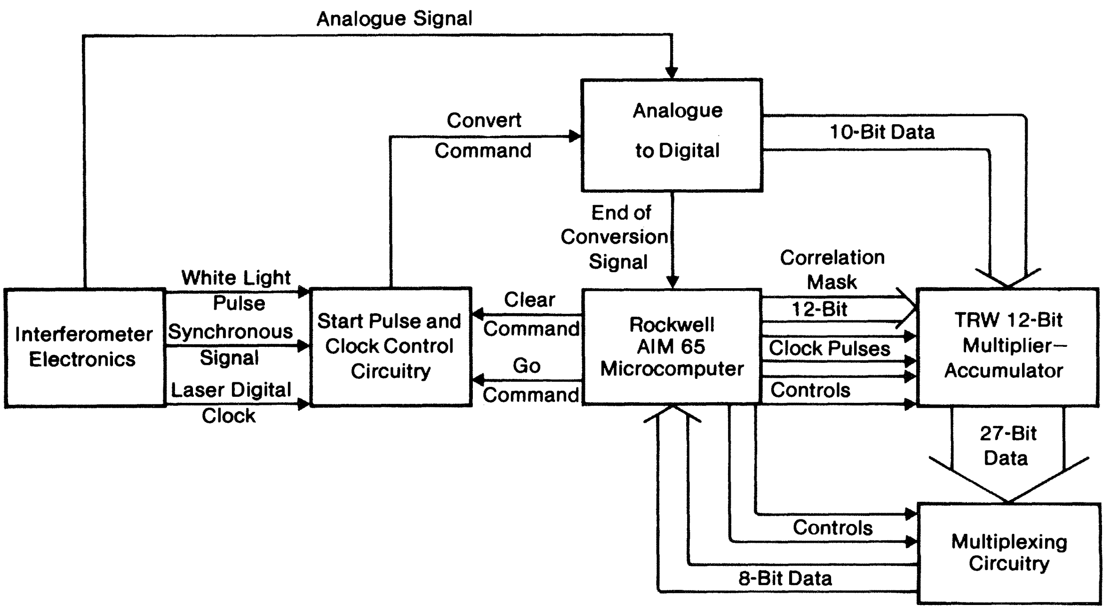

Figure 6. Block diagram for Rockwell AIM-65 microcomputer–TRW m.a.c. data-processing system for interferometric signals.

is processed by a software implementation of the fast Fourier transform (f.F.t.) algorithm to generate a conventional spectrum. This is shown on the left side of figure 5. The interferogram is for the i.c.p. atomic emission signal of a solution containing Na, K, Li, Rb and Cs. The interferogram and the processed spectrum contain 4096 data points; however, we only need information about the qualitative and quantitative presence of the elements in the original solution. About 70 elements have sensitive emission lines in the i.c.p. An alternative processing approach to the f.F.t. is simply to multiply the interferogram by sine and cosine waves corresponding to the frequencies of the most sensitive lines of the 70 elements. The summed products of the sine and cosine wave multiplications are then cominbed (root mean square) to form a single correlation data point indicative of the quantity of the required element present in the sample. The resulting output format of the information is shown on the right of figure 5 as a plot of correlation data points against element (Al to Zr). High correlation is clearly indicated for the elements known to be present. This process also amounts to a complete *automatic* computer interpretation of the spectral information. After the f.F.t. route we must still identify spectral lines; however, the correlation route directly indicates an element's presence without human interpretation.

The whole process outlined above can be implemented on a microprocessor system. A somewhat simplified approach based on the AIM-65 is shown in figure 6. The AIM-65 is only a controller and the heart of the system is a TRW multiplier–accumulator chip (m.a.c.) that performs in real time the complete correlation operation. The m.a.c. is capable of multiplying two 12 bit numbers and accumulating a 27 bit summation of such products. In the system shown in figure 6 the digitized interferogram is connected to one input of the m.a.c. and the appropriate sine or cosine function is fed to the other m.a.c. input from the AIM-65. After the correlation is complete (one cycle of mirror movement for the F.t. spectrometer) the correlation datum point is read into the AIM-65.

While this simple system is only capable of processing one frequency element at a time, it points the way to a simultaneous system consisting of a bank of m.a.cs, one for each element of interest, providing real-time readout of multi-element analytical data, or if the interferogram is stored in the AIM-65 it could be cycled several times to the m.a.c., each time being processed for a different frequency component. With the clocking rates of the AIM-65 and the TRW m.a.c., 70 elements could be searched for in a few seconds with appropriate element patterns stored in read-only memory.

Many more examples could be presented, but these two examples illustrate how inexpensive microprocessors and associated subsystems can be used to develop new instrument concepts.

An example from the consumer – small business – hobby market: the Apple II+

The foregoing examples of microprocessor-based systems used a high-level single-board system that is somewhat limited in capability compared with currently available consumer computers. Among the many systems now available the Apple, Commodore and Radio Shack systems are the most prominent, perhaps soon to be matched by the recently announced I.B.M. small business computer (Lemmons 1981).

In our own laboratories the Apple II+ system is being used. An average Apple II+ system consists of an Apple II+ (6502 central processor unit, 48 kbytes random access memory), a cathode ray tube monitor, two floppy disc drives (140 kbytes each), and a printer (Centronics 739). Such a system currently retails for about $4000. The Apple computer product is a good example of what can happen in support products when the system becomes widely accepted. As a result of the great number of Apple computers in use there has been generated a wide variety of sophisticated hardware and software products that directly and indirectly benefit laboratory data acquisition and processing. In many ways the indirect software developments are more important than the computer itself. A business man can walk into a computer store and upon seeing a demonstration of the extremely popular financial planning program VISICALC (reputedly the most successful program ever written) instantly buy $4000 of hardware to run $129 of software. It is this same market that is now providing extremely useful software and hardware for scientists that may in fact have been initially designed for small business or management situations. However, some laboratory-oriented hardware systems are available. Typical subsystems include analogue–digital converters, digital–analogue converters, clocks and digital input–output that can be directly plugged into the Apple. Often they are supplemented by rather complete demonstration floppy disc systems containing several programs that by themselves may completely solve certain data acquisition problems. For example, for about $600 from Interactive Structures one can get a 12 bit, 20 kHz, software programmable gain, 16 multiplexed input channel analogue–digital converter system complete with typical software programs on an Apple-compatible disc. Not very long ago, five to ten times that amount of money and several man months of programming would have provided about the same level of system for a minicomputer. In addition to demonstration software, some very powerful data processing software packages are available such as CURVE FITTER, VISICHART and SCIENTIFIC PLOTTER from Interactive Microware.

TABLE 3. APPLICATIONS OF DB MASTER

customer and client lists	supplier information
mailing lists	report generation
accounts receivable	label printing
inventory control	medical files
property management	research and reference data

Much of the support software available for the Apple is oriented towards the small business market; the main areas are financial planning, word processing and data-base management. Superficially one might think that these products are not readily applicable to laboratory operations. However, a program like DB MASTER from Stoneware is extremely useful. Typical applications of DB MASTER are summarized in table 3. In our own laboratory DB MASTER is used to 'manage' reference data. Quite extensive literature files can be maintained and automatically searched by several sophisticated modes. DB MASTER can be configured by the user for almost any laboratory data management task from reference data, analytical result data, research data, inventory data to mailing list data. It can be highly recommended, a $150 program that can save thousands of dollars in time.

In the domain of word processing programs, report generation, writing research papers, developing laboratory manuals, and writing letters and memos are all very time-consuming tasks for any scientist. Word processing systems are normally thought to relate only to office equipment, but the *individual* scientist may soon have to be completely familiar with the use of word processing systems because they will be part of scientific instrumentation as well as office equipment. To change the computer system from data acquisition, to data-base management or to word processing is simply accomplished by inserting the appropriate floppy disc and thus data-base management and word processing can be a normal component of an analytical instrument.

CONCLUSIONS

Some future or current trends are listed in table 4. Some of these have already been discussed and most were part of the scenario presented in the introduction. The availability of vast local memory facilities attached to the instrument or office is very important. Winchester discs are now available for the Apple with capacities of up to 20 megabytes allowing the equivalent of 67 floppy discs to be on line at the same time. Such local memory size allows very large scientific and personal data bases to be on line, e.g. complete infrared and mass spectral data files and extensive literature files. Video discs and tapes promise even larger data files. In addition to mass memory, the read–write memory directly addressable by the central processing unit (c.p.u.) will greatly expand as the 16 bit c.p.u's come into use with their 20 to 24 bit address buses. In addition to memory size, computing power will expand as array processors are developed for microprocessors. Voice input–output is here now. Both speech recognition and speech synthesis systems can be purchased quite economically. The Auricle I system can be trained by the user in a few minutes to recognize 80 words or short phrases. Complete voice input–output communication with a computer system is only a matter of time, awaiting imaginative implementation. Several examples of inexpensive sophisticated application software have already been cited. Suffice it to say that one must be aware of what is available and willing to adapt packages to uses perhaps not even imagined by the original program developers, i.e. business software in a laboratory instrument managing analytical data. The potential savings in man hours are difficult to overestimate. Finally, sophisticated portable computing power is now available. The Osborne 1 computer (briefcase size) includes a Z80 c.p.u., 64 kbytes of random access memory, two 100 kbyte floppy disc drives, a full keyboard and I.E.E.E. 488 and RS 232 interfaces, all for $1795. It is certain to have a major impact on the way in which anyone who deals with words or numbers works, at home, in the laboratory or somewhere in between.

Table 4. Future or current trends

1. vast local memory	4. voice input–output
2. vast computing power	5. sophisticated applications software
3. scientific or personal data bases	6. portable computing power

It is clear that the synergic action of current microprocessor subsystems will provide scientists with laboratory instrument and management systems that would have been incomprehensible only a few years ago. It is hoped that this discussion will inspire the reader to apply and develop imaginatively the computing power that is at hand thanks to the evolution of the microcomputer into a high-volume commercial product.

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