GENERAL PURPOSE MICROCOMPUTERS IN LABORATORY AUTOMATION

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Abstract - The general purpose microcomputer data system described was developed as a cost-effective means to bring the power of machine intelligence to a wide variety of one-of-a-kind chemical instruments and their researcher/operator. The salient design features include extreme low cost, modularity, optimized I/O structure for real time experimental control and data acquisition, economical large random access memory implementation, flexible video display generation for operator interaction and data presentation, hardware program bootstrap, compatibility with a host computer support system, as well as provisions for local mass storage and hard copy generation. Application to some specific instruments and its use as a stand-alone instructional unit are described.

INTRODUCTION

The microcomputer-based instrumentation automation system described here is an outcome of a continuing development effort in our laboratory to apply microprocessor technology to analytical instrumentation. Since its inception late in 1972, this effort has been directed at the investigation and design of microcomputer systems well suited to the general nature and requirements of contemporary and novel laboratory instrumentation and its researcher/operator.

DESIGN FEATURES

Some of the salient features of the resulting design are as follows:

1. Extreme low cost. If the computer is to become truly a commonplace measurement tool, its cost to the experimenter must be in line with existing general-purpose laboratory aids. A target figure of $1200-$1600 component cost for a basic but complete system for high-performance data acquisition and interactive analysis is achievable through microcomputer technology.

2. Modularity. A viable computer-assisted chemical analysis data acquisition environment is often characterized by a quite rapid rate of application turnover. Hence, a general-purpose data acquisition system is likely to be confronted by a succession of applications, each with differing requirements. A system configuration suitable for this environment must either be capable of handling most expected application demands in some standardized configuration, or else must lend itself with great ease to a "tailoring" process so that it may be "scaled" either up or down as the occasion demands. In an effort to maximize the potential efficiency of capital investment, the system described here exploits the latter method to an advanced degree.

Modular organization at the system-function level has been adopted to facilitate assembly of application-specific configurations. In this approach, high-level system components such as the central processing and system controller unit (CPU), large (16K byte) memory arrays, and peripheral input/output controllers are each implemented as single 4.5 x 10 inch etched-circuit cards. These units are interconnected <u>via</u> insertion into a parallel backplane bus, (which can accommodate up to 22 such units), to form the basis of complete systems.

3. Optimization of input/output structure for experiment control. Careful examination of
real-time applications in the chemical laboratory indicates that a small computer dedicated
to instrumentation will usually run out of response time and data acquisition speed capabi-
lity long before its computational capacity is exceeded. The computation associated with
experiment control is often trivial or even non-existent. What computation is needed is
usually associated with post-experiment data interpretation and need be completed only in
amounts of time commensurate with the patience of the operator. The speed of actual data
acquisition, however, is usually dictated by the physics of the system under study. Hence,
if the computer system is too slow in that regard, the work simply cannot be performed.

For these reasons, the design of a minimal cost data acquisition system must achieve a
highly versatile I/O structure possessing speed and generality for real-time operations
disproportionate to the computational power of the CPU. Instrumental control and data
acquisition related input/output has therefore received heavy emphasis in this system
design. This emphasis includes selection of an overall system design which includes
features useful in the provision of such functions [e.g. easily used direct memory access
(DMA)], the design of a large variety of standard "measurement-oriented" I/O modules, (e.g.
high performance analog-to-digital and digital-to-analog conversion and timing modules), and
the design of a system format supportive of implementation of specialized instrumentation
interfaces, (e.g. provision of well-regulated standard supply voltages, and adoption of a
popular circuit-card format insuring commercial availability of prototyping hardware).

4. Economical, expandable implementation of large random access memory arrays. Analysis of
various categories of measurement-automation applications reveals frequent requirements for
"memory-intensive" system designs - either due to large control programs or the generation
of extensive data arrays. 4K dynamic memory components were therefore chosen in the UNC-
chem design as the basis for main system storage because of the superior cost, space, and
power requirements of these units (less than 1/4 cent, 3.5×10^{-4} square inches, and 80
micro-watts per bit, respectively), when compared to any currently readily available competi-
tive technology.

Memory systems utilizing dynamic chips must, however, incorporate some technique for pro-
viding the periodic refresh activity needed to maintain the integrity of stored data. The
methods used to implement memory refresh in most micro-computers using the dynamic techno-
logy may be characterized as asynchronous in the following sense: In generally used refresh
techniques, necessary refresh cycles are "stolen" from normal memory activity upon demand
from a free-running timing circuit. These stolen cycles occur independently of other
system activities and are, thus, asynchronous to those activities. In the general run of
micro-computer applications, this method of memory maintenance is simple to implement and
efficient in terms of average memory availability. A difficulty arises, however, in the
context of high-performance instrumentation control from the following circumstance: If,
in the course of system activity, a memory access request (as might be generated in an
attempt of the CPU to fetch an instruction) should occur simultaneous to a refresh cycle
"theft", asynchronous refresh logic would defer granting of the system access request until
the refresh cycle was completed, thus anomalously increasing (usually doubling) the time
needed to satisfy the deferred request. Because such conflicts occur unpredictably during
the progress of experiment control, unavoidable timing indeterminacy is introduced into
computer/instrument transactions. While the resulting indeterminacy is small, and thus
inportant only for relatively high-speed experiment control, the performance we desired for
the UNC instrument made it intolerable.

This effect is avoided in the UNC micro-computer system by two measures. First, timing for
refresh is derived directly from the main system timing reference and is thus synchronous
with all other system activity. Secondly: refresh is performed at an average rate far
higher than specified by the memory-chip manufacturer as needed for the maintenance of data
integrity. This fact allows memory access for refresh to be given a priority lower than
that given CPU and I/O-originated requests. Thus, in the event of an access conflict, it is
the refresh request that is deferred guaranteeing that the experiment-related transaction
will always proceed on schedule. The very high average rate of refresh insures that, even if
a large number of such refresh-cycle denials occur, data integrity will not be threatened.

5. Flexible video display generation is incorporated as an integral function of the CPU
module. Effective interaction of the researcher with computer-controlled instrumentation is
dependent upon timely and meaningful presentation of acquired data and experiment status.

One of the most consistently successful means of data presentation is the CRT graphic display. Early in the design of this microcomputer system, provision was made for an economical graphic display with useful resolution using low cost video monitors (or even lower cost consumer-grade TV's) as the display medium. Display format is a 256 x 256 point map, permitting presentation of both graphic (e.g. spectra) and alphameric (e.g. system messages and numeric tables) data. Central to the feasibility of this display design approach, (due to the need for a 65,536 bit memory area for service as an image buffer) is a method for efficient implementation of large memory arrays. Use of dynamic 4K MOS memory components yields a display-related memory cost of $80 at current prices. That figure, when combined with the cost of a suitable monitor and other display hardware, leads to a total cost for this versatile operator interaction resource of under $200.00. At this level of expense, graphic display capability becomes economic as a universal basic peripheral of low cost systems. An interesting feature of display generation is that memory references needed for display maintenance are simply those occurring in the course of memory refresh. The 4K memory devices used in system memory (Intel 2107B or Texas Instruments 4030) are of a variety refreshed by the execution of read cycles. Refresh maintenance, therefore, is performed very well simply by the previously described memory activity associated with display generation. Thus, the television is driven largely by logic which would be needed in any case merely to preserve memory contents. The only additional circuitry needed consists of an eight-bit shift register to serialize the video output, and provision for T.V. synchronization-pulse generation.

6. Compatibility with a host support system. Because the UNC-chem micro-computer was configured from the outset to be well suited for duty as a component in a multi-laboratory system, features have been incorporated in its design to facilitate such operation. "Bootstrapping" of the terminal computer into operation from a host system (i.e., initial loading of controlling programs), transfer of data acquisition control programs from the host library, data transfer, and other facets of computer-computer communication are easily and efficiently performed.

7. Hardware-implemented program bootstrap. Because of the envisaged rapid turnover of application programming, all of a micro-system memory is composed of read-write storage, rather than partly read-write and partly read only. This organization provides maximum flexibility in program implementation and change. However, an obvious requirement is generated for a means of initial program entry in the event of memory loss. The availability of the program-independent DMA input-output, combined with a small amount of additional circuitry, permits the UNC micro-computer prototype to accept initial program input from a variety of sources including cartridge or cassette mag-tape, teletype paper tape reader, or a supporting host computer. Specific "bootstrap device" selection is accomplished by a jumper wire connected from the CPU card to the appropriate device controller. The bootstrap or FILL mode is initiated automatically upon power up, manually, via a front-panel switch, or under program control. The FILL mode is terminated by end-of-record status within the bootstrap device controller.

HARDWARE COMPONENTS

System elements and modules of the UNC-chem microcomputer system group naturally into a number of functional categories, although a single component will occasionally offer utility in, and therefore logically belong to, more than one grouping. A listing organized in this fashion of available system elements including approximatel cost, construction effort (in man days), and functional description, follows.

Central processing components
1. System housing ($180, 2 m-d). Built entirely from commercially available modular components, the system housing includes power supplies, card guides, connectors, and backplane bus.

2. CPU card ($175, 1.5 m-d). Carries 8080A microprocessor chip and performs functions associated with microprocessor support, bus management, Direct Memory Access, Video Display generation, memory control and initial program load (automatic bootstrap).

3. 16 K-byte RAM card ($160, 1.0 m-d). Carries 32 4K by 1 bit dynamic Random Access Memory devices (Intel 2107B or similar) to provide 16384 bytes of power-conservative program and data storage. High-order address decode is provided to permit up to 4 RAM cards to

co-habit available address space for a maximum system memory of 65,536 bytes. Read cycle time is 750 nsec, write cycle is 1500 nsec.

Real time data acquisition and experiment control

1. **Successive approximation ADC card** ($130, $170, or $270, 0.75 m-d). Accepts any one of a series of pin-compatible 12-bit ADC modules of differing maximum speeds (DATEL ADC-H series) to support 12-bit throughputs of 45K to 330K conversions/sec and 8-bit throughputs of 57K to 430K. Control signals are provided for up to 16 channels of parallel track/hold and for interface to the high-speed averager card. Provision is made for use of this ADC card with the I/O sequencer module.

2. **Quad track/hold card** ($135, 0.75 m-d). Implements 4 independent track and hold amplifiers with associated analog multi-plexing so that, at the onset of a conversion scan cycle by the ADC card, all four input signals are simultaneously captured and sequentially presented to the ADC for conversion. Up to 4 such cards, for a total channel count of 16, may be connected to one ADC. Specifications include acquisition time of 3 usec to 0.01%, aperture uncertainty of 20 NS, and multiplexor delay of less than 1 usec to 0.01%.

3. **Hardware averager card** ($40, 0.25 m-d). This card implements a direct interface to the ADC by means of which 8 bit conversions may be added to (or subtracted from) multiple-byte-precision memory accumulations. In this way, enhancement of experimental-data signal/noise ratios may be achieved through ensemble averaging. 8, 16, 24, or 32 bit sums may be computed with number of summation bits, as well as selection of addition or subtraction, under program control. Time required for summation update is 3 usec/byte.

4. **High speed I/O sequencer module** ($55, 0.5 m-d). This card provides a versatile means of generating time-related sequences of computer-experiment interactions through direct memory access at speeds far exceeding the capabilities of the micro-processor to manage such activity. The I/O sequencer utilizes a 16-bit variable modulus counter driven from the 2 MHz system reference to control timing between experimental "events" with an accuracy of 0.01% and a resolution of 0.5 usec.

Upon expiration of an inter-event period (as determined by overflow of the counter or by receipt of an external trigger), initiates the generation of a sequence of up to 8 I/O control pulses. Pulses appear on individual points available on the sequential programming module and are routed to those elements in the controlled instrumentation system which are to participate in the I/O program.

For any given event a subset of the 8 pulse lines are selected for actuation by an 8-bit program mask byte loaded into the program shift register from microcomputer memory during the interval between events. In addition to sequencer operation, this module can also be used as a 16 or 32 bit event timer.

5. **Quad 12-bit DAC** ($165, 0.5 m-d). Four 12-bit, independently latched analog output channels are provided by this card. Approximately 5 usec are required for the re-load and settle of any channel (under DMA). The transfer of new 12-bit values to the DAC buffer register are performed as parallel "jam" transfers so that output "glitches" are minimized. Operation under I/O sequencer control is possible. The inclusion of a plotter-pen control bit on this card makes it useful as an XY plotter interface. Select address strapping permits up to 4 of these quad DAC modules to co-exist in a single system.

6. **Integrating ADC and 20 Hz clock** ($60, 0.5 m-d). This peripheral implements three channels of 16 bit resolution, auto-zero-compensated analog to digital conversion with a maximum aggregate throughput of 20 points/second. The span of each channel may be selected (via input resistor network) independently of the other two. Inputs are fully differential (60 db common-mode rejection) with a 100K ohm/volt impedance and high "survivability" (i.e. application of 110 VAC to inputs without damage). Normal-mode rejection of 60 Hz-related noise is greater than 66 db (limited by power-utility frequency accuracy).

Operator interaction and data presentation peripherals

1. **Video display (TV)** ($100, 0.25 m-d). The major medium available for immediate

communication to the operator of system and experiment status and data is a 12-inch video
display implemented via a consumer-grade solid state television receiver modified to accept
ElA-standard composite video (or, equivalent but more costly, a standard CCTV monitor). The
output medium so implemented is both a graphic display of 256 x 256 resolution and an alpha-
meric display with a format of 42 lines of 64 characters each (2688 chars. total). Graphics
and alphameric text may be freely mixed. Display "polarity" (i.e. white-on-black or black-
on-white) is program selectable.

2. ASCII keyboard ($160, 0.06 m-d) and controller ($25, 0.2 m-d). A parallel-interface
ASCII keyboard (Cherry Inc. #B70-61AA) with companion controller module, this peripheral
provides a flexible means for input of operator commands to the microcomputer. The con-
troller will support a variety of parallel keyboard interface requirements.

3. Teleprinter ($800-$1800) and interface ($25, 0.25 m-d). The wide variety of available
teleprinter terminals affords the basis for flexible operator communications where hard copy
is desired. The interface implements a general purpose asynchronous serial link (UART-based)
and accepts 20-m.a. current loop or RS232-standard signals of 110, 300, 600, 1200, 2400,
4800, or 9600 baud. All common character formats are accomodated.

4. Miniature line printer ($450, 2 m-d). This peripheral utilizes a 3.5" line width, dot-
matrix, impact print mechanism (LRC Inc., #7040) to implement a 150 line-per-minute, 64
character-per-line, bidirectional line printer.

5. Electrolytic facsimile recorder ($850, 2 m-d). Based upon a six-inch electrolytic-
marking raster-scan recorder (Alden Inc. #600), this peripheral provides an efficient means
for both graphic and alphameric output. A number of operating modes are possible, one being
the use of the fax recorder to generate hard copies of the video display – a process
requiring approximately 20 seconds and $0.01 worth of the electro-sensitive paper.

6. XY recorder ($1100, 0.5 m-d) and controller ($105, 0.5 m-d). Software has been developed
which permits the use of standard analog XY recorders (Hewlett Packard Inc. #7040) as ver-
satile generators of annotated graphical hard copy.

Magnetic media storage
1. 1/4" Data cartridge drive ($700, 1.5 m-d) and controller ($70, 1 m-d). This peripheral
provides a high-performance medium for rapid storage and retrieval of system programs and
experimental data. Chosen as the basis for this important system resource is the 3M DC-300
data cartridge used with a Mohawk Data Sciences 2021 transport and in-house read/write,
motion control, and formatting electronics. In this system, the recording medium is
formatted as a directory-driven random access storage area within which as many as several
hundred files may be accessed by user-assigned alphameric names of arbitrary length. Files
may consist of any number of variable length records up to a maximum of 700K bytes per file.
Total cartridge capacity is 2.8 mega-bytes organized as 4 independent tracks. Provision is
made on the controller card for the management of up to 4 transports-yielding the capability
for an on-line capacity of up to 11.2 M-byte. Recording density is 1600 bits/inch and data
transfer occurs at 6K bytes per second. During recording, a read-while-write check is
performed of data record integrity. Worst-case random-access delays are proportional to the
fraction of cartridge storage capacity utilized and are approximately 30 millisec. per
K-byte. Thus, access times over a 200K byte system would not exceed 6 sec. This figure is
subjectively comparable to the 1.3 sec worst-case figure derived for a typical floppy disk
(Memorex 651) performing a similar directory-driven random access over 200K byte. Worst-case
sequential access delay is approx. 30 milli-seconds for the cartridge against 160 milli-
seconds for a floppy disk.

2. Audio cassette recorder ($35) and controller ($40, 0.5 m-d). Based upon a simple FSK
(1200/2400 Hz) extremely speed-tolerant ($\pm$50%), synchronous data encoding format, this
peripheral allows the reliable storage and retrieval of substantial data/program files (up
to 1.4 megabyte per C120 cassette – both sides unformatted) at respectable speed (200 bytes/
sec.) using entirely unmodified consumer-grade audio cassette recorders. Sequential access
delay is 3 seconds maximum (recorder start/stop time). Random access by file name ranges
from tens of seconds to tens of minutes depending upon cassette utilization and the amount
of manual intervention supplied by the operator in the form of fast forward tape movement,
etc.

Communication with shared-resource computing hardware
1. Parallel digital communication (Lab-box) interface ($40, 0.5 m-d). Much of the
development of UNC-chem micro-computer software has been performed using available Raytheon
minicomputers in the role of cross-assembly and linking down-load processors. The ability
to make use of convenient source-handling peripherals (card reader, line printer) has proven
to be a great asset. In addition, the use of minicomputer-maintained magnetic disk memories
as program libraries and mass data storage has been invaluable (particularly before the
availability of magnetic media priced compatibly with the microcomputer) as has the ability
to access shared minicomputers as computational resources.

The Lab-box interface implements the micro-computer side of a digital communication link
providing a 10K byte/sec, automatic error correction via retransmission, down-load, and
cold-start (bootstrap) capabilities.

2. Asynchronous serial interface ($25, 0.25 m-d). An alternate means of computer/computer
communication is provided by this module. 20 ma. current loop, RS232 and TRL compatible,
the serial interface supports full-duplex communication at rates up to 9600 baud via direct
wire or modem link.

3. Stream-multiplexed, packet-oriented serial link ($50, 0.5 m-d). This module implements
the microcomputer side of a ring-organized, integrated communication system designed for a
hierarchical multilaboratory computer network with the following properties:

Handles all system communication via one party-line cable;
Bit-serial;
Undirectional data flow (circular bus topology);
Data and control are transmitted in 15-bit "packets" at 1.5 mega- baud to achieve a net
transfer rate of 100K Byte/sec;
End-to-end error control is maintained in all bus activity;
Connection of terminals to bus is via signal-regenerating "T-TAP"/repeaters - allowing
virtually unlimited cable length and number of terminals;
Ground isolation (pulse transformers in taps);
Selection of terminals by host-computer polling;
Polling transaction is one 10 micro-second packet.

SOFTWARE DEVELOPMENT TECHNIQUES AND RESOURCES

Crucial to the utility of any computer system is, of course, the ready availability of
effective means for the development, de-bug, and access of general-purpose and application-
specific software. Major categories of software support needed for the full and efficient
utilization of computer techniques are:

1. Machine-oriented-language software development (assemblers)

2. Macro-level utilities (floating-point and multiple-precision arithmetic, trancendental
    function packages, I/O handlers, I/O formatters, graphic-output generators, command-
    string parsers, etc.)

3. General system utilities (text handlers and editing resources, relocatable and memory
    image libraries and loaders, linking load-module generators, general file maintenance,
    etc.)

4. Problem-oriented-language software development (compilers, interpreters).

Early in the organization of the UNC-chem microcomputer effort, the decision was made to
design our software development resources around available mini-computers in order to take
advantage of convenient text-manipulation peripherals (card readers, high-speed printers)
attached to those machines. In addition, disk-memory-based library processors were
available on these machines which promised powerful facilities for maintaining extensive
linkable, relocatable files of macro-level microcomputer utility packages. Accordingly,
software was developed to exploit this ready resource consisting of:

a. A package of assembler macros (180 source lines) was written to define the micro-computer

instruction set to the existing minicomputer assembler. Thus was that processor
converted, with minimum effort, into a cross-assembly program which naturally produced
object text compatible with the minicomputer linking loader and library processors.
Those extensive programs were therefore also made useful in microcomputer software
development and access.

b. A down-load processor was written to relocate code linked by the minicomputer linking-
    loader and transmit it to a target micro.

c. An I/O driver was coded for the minicomputer to facilitate minicomputer-microcomputer
    communication.

d. A number of specialized library-manipulation programs were written and integrated into
    the minicomputer executive to facilitate microcomputer-configuration-specific down-load
    and bootstrap parameterization.

Using the resources so provided (comprising about 2400 source lines in all), the UNC group
proceeded to code the extensive software support components and utilities of categories 2, 3,
and 4. At the date of this writing, approximately 17,000 source lines of such code has been
generated providing a rich environment for the development of applications software. Among
the tools produced in this way is included a BASIC interpreter possessing a unique combination
of data-file and graphic image manipulation capabilities. The BASIC language has proven to
be a useful resource for both the instructional environment and for researchers unfamiliar
with the powerful but arcane methods of the assembly-level programmer.

APPLICATIONS

Having developed the hardware and software generation modules to the point where ready
replication of the microcomputer units themselves was feasible and software generation had
higher level support, our attention has turned to the various specific applications
described here.

Control, data handling and analysis system for ESCA. The x-ray photo-electron spectrometer,
while a powerful analytical tool of rapidly increasing popularity for surface characteriza-
tion, may be limited in versatility and throughput by association with an inflexible data
management system. In this laboratory, for example, a Dupont 650 spectrometer interfaced
to and controlled by a 1024 word Nicolet Multi-channel Analyzer was used to perform ensemble
averaging of repeated energy scans, data enhancement (usually simple 3-point smoothing),
and output of acquired spectra onto an X-Y recorder. While a reliable, easy to use instru-
ment, the Nicolet MCA suffered from a number of inherent deficiencies which limited both
efficiency of utilization of the spectrometer and the sophistication of data treatment.
The multi-channel analyzer was capable of only simple linear scans of specified energy
regions at a fixed time (0.1 sec.) allotment per unit (50 mV to 1V) energy interval. Hence,
if a number of disjoint energy regions must be scanned to characterize a particular sample,
each region must be dialed in and run individually by the operator. Besides adding the
time required for each interval initiation to that required for actual data acquisition
and thus reducing sample throughput, this instrumental shortcoming also complicates the
analysis of samples which undergo surface changes during x-ray exposure. Because each
individual energy interval was effectively taken with a significantly different cumulative
x-ray exposure, considerable operator wariness was needed to avoid taking invalid data.

A substantial improvement in spectrometer utilization and data quality resulted from inter-
facing a microcomputer to the ESCA spectrometer. Particularly important is the capability
to scan a disjoint set of independent regions with ensemble averaging occurring over the
entire set. In addition, a variety of mathematical data enhancement and interpretation
aids can now be brought to bear upon acquired spectra, features previously limited to the
algorithms "hard-wired" into the MCA. Valuable schemes include peak de-convolution to
remove effects of the non-monochromatic x-ray source, background subtraction, area determi-
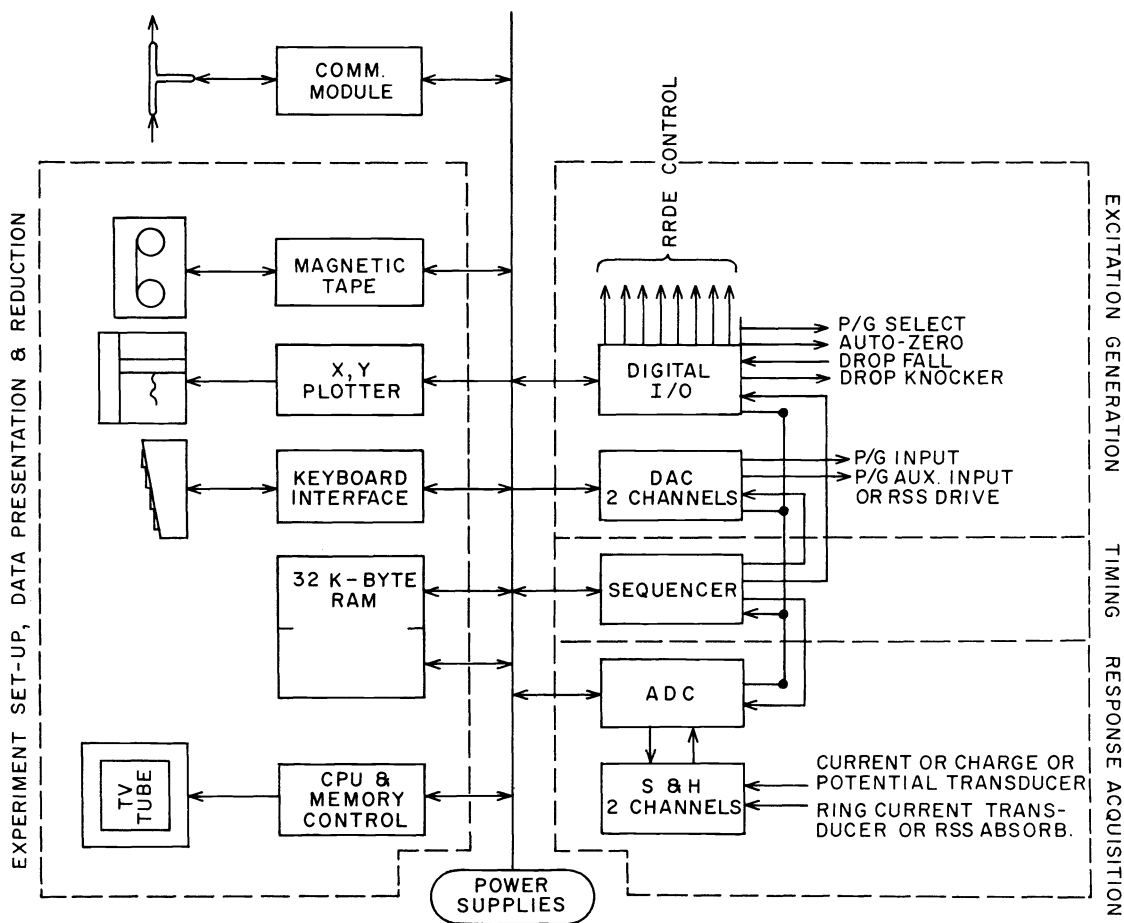nation, superior graphics, data storage and retrieval of data, and band-fitting capabilities.

Fig. 1. ESCA Configuration

As indicated in Fig. 1, only two special purpose cards were added to a standard configuration UNC microcomputer to achieve the desired system. One card is a high precision (16-bit) DAC which controls the analyzer voltage. The other card contains two functions, a 16-bit pulse counter and a 8 usec. resolution time base (clock). The pulse counter accumulates amplified detector pulses until interrogated at the end of a timing interval which is controlled by the 16-bit programmable clock.

The interactive software program was written in 8080 assembly language. To facilitate use of the ESCA by the many different and sometimes infrequent ESCA users, the commands were kept simple and included checks for illegal entries. The five groups of commands are initialization, acquisition, display, data handling and data storage. The operator may select up to eight binding energy regions (frames) to be acquired in one experiment specifying the initial binding energy, the scan range, the resolution and the number of scans for each frame. The only restriction is that the total number of points acquired must be less than 5500. Acquisition proceeds sequentially through the frames acquiring one scan per frame until all the initialization conditions are satisfied. The data is auto-scaled to maintain 2-byte sums and displayed in real-time. Following acquisition one to four frames may be displayed on the TV or plotted. The data handling routines include removal of the effects of the Mg $K_{\alpha3,4}$ lines in the non-monochromatic x-ray source, three-point smooth, background subtraction, charging effect correction, expansion of a frame, integration and cursor readout. The data may be stored on the 3M magnetic tape cartridge and retrieved at a later time for further data processing and/or plotting. The data can also be accessed from the tape by other programs. One such program reformats the data in a form compatible with the BASIC interpreter and writes it back on a tape. This allows users to write their own data manipulation procedures in BASIC. This type feature is quite useful for handling special problems which occasionally arise and can be performed
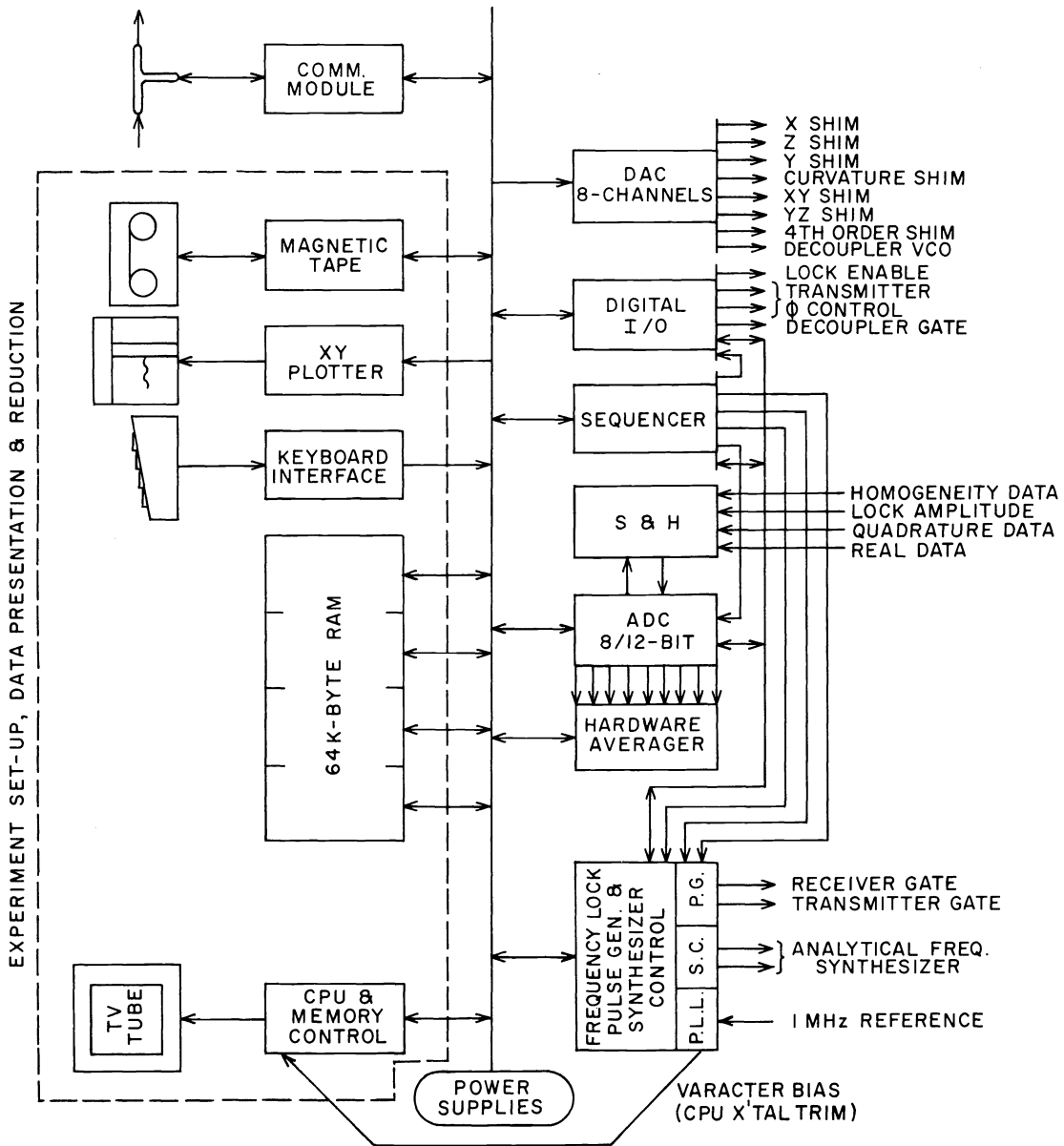
Fig. 2.   Configuration for multi-nuclear F.T. NMR spectrometer

micro-computer action and the R.F. circuitry of the spectrometer, the 16 MHz internal clock of the micro is synchronized with the 1 MHz master reference of the spectrometer frequency synthesizers via a phase lock loop controlling the varacter bias in the CPU crystal oscillator.

The multinuclear F.T. NMR spectrometer was assembled in our laboratory around a HA-100 magnet/probe system, replacing the HA-100 continuous wave gear with commercially available modular R.F. components.

The observe circuitry is broadbanded excluding the probe components. State of the art commercially available mixers, phase shifters, quadrature detector and IF amplifiers are used along with a frequency synthesizer and 100 watt broadband transmitter to compose the RF observe section. The audio portion contains twin audio amplifiers and computer controlled Butterworth filters. The system utilizes an internal deuterium lock with RF

by the user who can be expected to know a high level language. Another widely utilized
program is a curve-fitting routine which decomposes a spectrum into a specified number of
peaks using a nonlinear residual least-squares technique. The function used for
approximating an ESCA peak consists of a weighted Gaussian-Lorentzian peak plus a sigmoid
background. Six parameters define the function: the height, position, and width of the
Gaussian-Lorentzian curve, and the height, position, and slope of the sigmoid. The
fraction of Gaussian character is specified by the operator but not varied in the fit.
A linear baseline of variable height and specified, fixed slope is added to the sum of all
the peak shapes to produce a calculated spectrum, which is compared to the actual data.
Marquardt's method is used to modify the peak parameters iteratively to achieve the best
fit. As the computation proceeds, the calculated spectrum is displayed on a TV screen
along with the data, to facilitate operator interaction. When the fit is complete, plots
of the data, calculated spectrum, and individual peaks and sigmoids are available, as is a
printout of the area under each peak. Other program options include background subtraction
and smoothing of data, and selection of parameters to be held constant. A similar routine
written in FORTRAN for a minicomputer was earlier utilized for this purpose. The program
was rewritten in 8080 assembly language by David Smith for the microcomputer, and is
approximately 15K bytes in length. Interestingly the microcomputer program's speed and
performance are comparable to the routine written in FORTRAN and run on a minicomputer;
the graphics capabilities and ease of operation of the microcomputer version are superior.
Our experience shows that curve-fitting, a sophisticated mathematical procedure, can be
handled readily by an inexpensive microcomputer.

Multi-nuclear F.T. NMR spectrometer. The management of the data production of pulse NMR
spectrometers is an instrumentation automation problem of interesting diversity. Detector
sampling rates of up to 100 KHz are required to characterize spectra containing large
chemical shifts. Multiple transients must be averaged to overcome the low signal-to-noise
ratios produced by low-sensitivity nuclei. Many thousands of data points are required to
achieve high resolution spectra. Many channels of spectrometer control signals are required
for such functions as homogeneity optimization and frequency selection. High speed control
lines possessing a stable phase relation to system frequency references are needed to
generate transmitter excitation pulse sequences.

The above functions must be abdicated to the spectrometer throughout the capture of a
given data set - often a period of hours. Once the raw ensemble averaged transient has
been acquired, processing, in the form of Fourier transformation is required. The latter
computational step, while of considerable complexity and requiring the attention of at
least a moderate size minicomputer, can generally be completed in a time short compared to
that required for the original data capture. Thus the image which emerges of free induction
decay spectroscopy data management is one of a demanding, long term I/O interaction with
the experiment, followed by a complex but brief computational requirement. Such a combina-
tion is a natural for a apparatus comprising a micro-computer instrumentation system and an
associated mini-computer number cruncher which could be shared with other instruments and
users.

The relatively stringent demands of the NMR application results in a "stuffed" micro-
computer configuration as indicated in Fig. 2.

Memory configuration is a full 64K to permit 16K sample data sets at multiple byte pre-
cisions. Data capture is performed by the standard 12 bit, 3 bits/µsec. ADC and is capable
of operating in two modes. For single transient acquisition of high S/N signals, the ADC
may be operated in the usual fashion acquiring 12 bit samples. In the capture of lower
quality signals, however, the ADC is utilized with a hardware averager card which adds the
high order 8 bits of the conversion result to an ensemble sum of 8, 16, 24, ... or 64 bit
precision. Addition time is 3 usec. per byte. In this way variable resolution data
averaging directly to memory is achieved at rates up to 100 KHz. In either mode, a two
channel sample-and-hold/multiplexer card is used to simultaneously acquire both in-phase
and quadrature detector outputs at the onset of each sample time. In addition, two other
channels are provided to monitor both a total transient energy channel, as a measure of
magnet homogeneity, and a lock amplitude channel to measure lock performance.

System timing, including controlling pulses to the sample excitation transmitter, is
generated by a standard sequencer card. In order to maintain precise phase lock between

detection similar to the observe circuitry. The lock phase detector provides the appropri-
ate error signal to the magnet's flux stabilizer. Broadband decoupling is accomplished by
square wave phase modulation a frequency synthesizer and a 10 watt broadband amplifier.

Special features include CAPS (computer alternating pulse sequence); homospoil option;
interchangeable lock and observe probe preamplifiers and transmitter matching networks;
computer controlled frequency synthesizer, Butterworth filters, 0 to 360° RF observe phase,
and pulse gating; a high power output gate for the observe transmitter; and BNC connector
uniformity for each module, most of which are commercially available, allowing for user
analysis and replacement. A single temperature controlled crystal oscillator is utilized
for establishing a common time base for the observe, lock and decoupler channels as well as
for the microcomputer.

The system software is written in 8080 assembler language and supports all hardware functions
including CAPS, homospoil, and host processor communications. Operator communications and
graphics are via keyboard and video display or X-Y plotter. Data analysis software includes
full phase correction for up to 8K complex pairs and peak location routines.

In an earlier configuration, a high-performance minicomputer, Mod Comp II, was dedicated to
the NMR instrumentation during data acquisition and reduction, and hence was not available
for other data acquisition or computations in our laboratories. In the current micro-
computerized version, the mini-computer now serves as a host processor to the spectrometer
microcomputer for Fourier transform computation and microcomputer software development, and
hence is more available for the general laboratory uses.

Stand-alone instructional microcomputer. Because of their low cost, effective TV graphics,
and availability of a high level language, BASIC, the use of stand-alone configurations
for educational purposes appears quite feasible. Fig. 3 illustrates the unit used for
this purpose. Without the optional hard copy peripherals, the hardware cost is $1035.

The BASIC interpreter resides on an inexpensive consumer grade audio cassette tape and can
be booted into memory and brought into execution by the clear-fill switch within 40 sec.
The student can then compose programs using the keyboard as input and the TV for alpha-
numeric output. Programs so constructed can be saved on an audio cassette and reloaded
when desired. In this way the student maintains his own programs. Data can be handled in
the same manner. One unit in the laboratory is provided with hard copy output so that
listings can be provided for debugging efforts away from the computer. A number of
students have learned BASIC simply by being provided with access to the instructional unit
and given a copy of one of the many BASIC textbooks. It seems clear that microcomputers in
this form will eventually be installed in large numbers in high schools for educational
purposes. The unit is quiet and avoids the relatively high charge of time-sharing services.

The instructional microcomputer was recently used in our 5 week short course on numerical
analysis, which meets one afternoon each week. A broad outline of its coverage is given in
Table 1.

For the laboratory phase of the course, the students were assigned various chemically
oriented projects to solve, each requiring the use of one of the topics in Table 1. They
were also furnished cassettes containing canned suboutlines in BASIC language and often a
primitive driver routine for illustration. The student had to write a suitable driver
program for his chemical problem and to furnish a copy of his final program on a cassette to
the instructor for grading purposes.

Topic 6 on Fourier transforms and time series analysis was handled in a somewhat different
way. A second year graduate student, Gene Woodard, wrote a rather eloquent, interactive
BASIC program, which was simply loaded in and run, and an accompanying manual described
its use. This demonstrator program illustrated the properties of various Fourier transform
pairs, utilizing pulses, sampled sinusoides, etc. and computed the corresponding complex,
power, and linear spectra. Heavy use was made of the graphics capability to draw annotated
pictures on the TV display. Other subjects included were waveform analysis, convolution,
auto- and cross-correlation, leakage, apodization, and filtering via manipulations in the
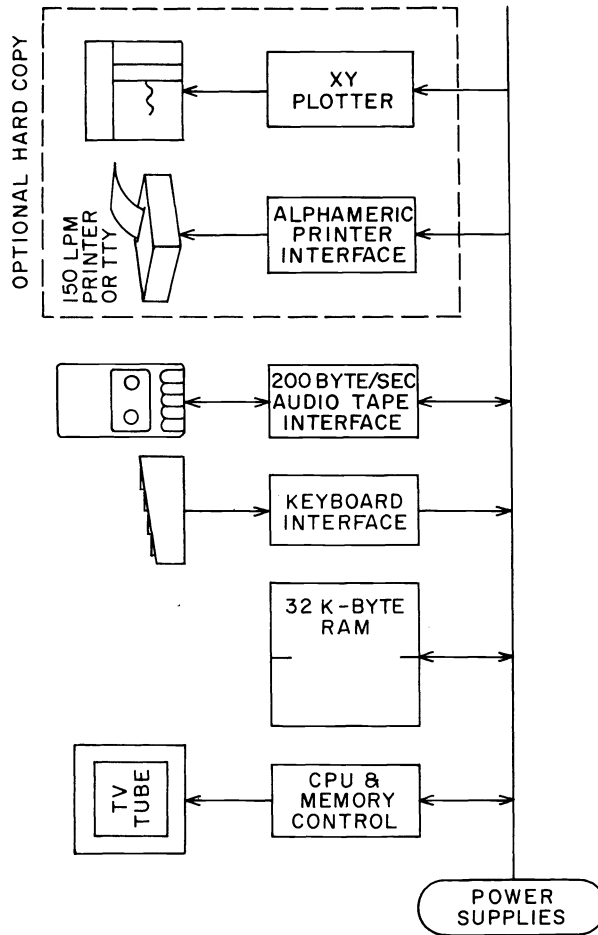frequency domain.

Fig. 3. Configuration of stand-alone instructional microcomputer

TABLE 1. Topics in numerical analysis

1. Matrix algebra; linear simultaneous equations

2. Approximations and interpolations (polynomials)

3. Finding roots of a single equation

4. Numerical integration and differentiation

5. Numerical solution of ordinary and partial differential equations

6. Fourier transforms and time-series analysis

7. Digital filters

8. Simplex optimization

9. Non-linear least square fitting

10. Multivariate analysis

In the future we anticipate incorporating one integrating ADC/20 Hz clock card and one quad 12-bit DAC card and adding the relevant statements to our BASIC language so that these instructional units could then be utilized in the data acquisition and analysis short course which occurs after that on numerical analysis. Also the development of a suitable stand-alone assembler would permit the use of the instructional microcomputers in an assembly language short course and in teaching interface techniques (hardware and software).

APPLICATIONS IN PROGRESS

In an earlier application survey (1, 2), we concluded that the microcomputer, with a suitable design architecture, could be an effective intelligent terminal in a wide variety of chemical instrumentation environments. Some of these additional areas of application which are receiving current attention are described here.

Search systems. Currently the UNC microcomputer is being programmed to handle spectral search problems. An essential ingredient to this work is the availability of the high performance magnetic cartridge storage with its 2.8 mega-byte storage capacity. This is sufficient to store ~ 95,000 binary infrared spectra on a single $20 cartridge without further data compression. A study of ~ 2000 carbon-13 NMR spectra indicates that 9-bytes per spectra would be required, leading to the possibility of storing ~300,000 compressed spectra on a single cartridge - a figure which far exceeds the availability of such spectra at the current time. Another area being pursued is low resolution mass spectra.

Universal programmable electrochemical system. The ability of the UNC microcomputer to provide highly accurate time-correlated experiment-control functions will be utilized in this application to configure a highly flexible instrumentation system capable of per-
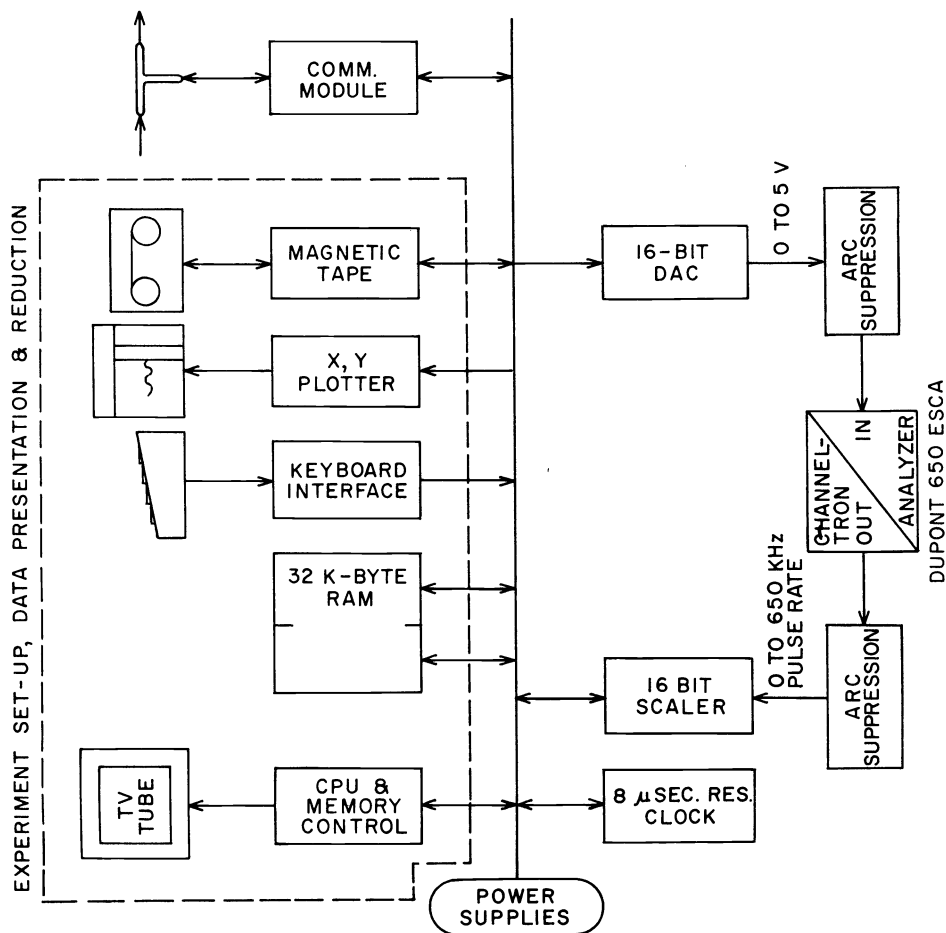

Fig. 4. Configuration for electrochemistry

forming a wide variety of experimental electrochemical techniques. This proposed instrument system will comprise three main functional blocks: a) experimental system excitation and control, b) response transduction, digitization, and acquisition, and c) data presentation and reduction.

The system will be packaged as two major pieces, namely the microcomputer and an electro-chemistry panel. The microcomputer bay will contain the modules shown in Fig. 4.

The electrochemistry panel will mount electronic components (operational amplifiers, analog switches, driving circuits) arranged in functional blocks designed to permit the quick and convenient implementation of electrochemical apparatus. The range of capabilities will be sufficient to perform, when driven by excitations generated by the controlling micro-computer, most commonly encountered electrochemical techniques without requiring additional electronic instrumentation. Provisions will include:
1. Galvanostatic and potentiostatic modes.
2. Three and four - electrode potentiostatic systems featuring control amplifier compliance of $\pm$ 100v and transient current levels of up to 0.1 ampere.
3. Simultaneous current and charge monitoring in one and two working electrode potentio-static systems.
4. Automatic zeroing of instrumental offsets; e.g., transducer and integrator errors in potential step chronocoulometry.
5. Optical drop-fall detection for DME.
6. Electro-mechanical drop knocking.
7. Digital control of rotational speed in "ring-disk" experiments.

Besides providing for facile implementation of a variety of electrochemical techniques, the design of the panel minimizes the use of manually set potentiometers as a method of parameter entry. The expense, frequency characteristics, and limited accuracy of these common devices will be avoided whenever possible through the substitution of computer scaling of electrical parameters. Operator interaction with the experiment will be mediated by a combination of graphical and keyboard-oriented input techniques designed to duplicate the immediacy and naturalness of "knob-twiddling" without the afore mentioned limitations of potentiometers.

Support programming for the electrochemical system will emphasize modularity to both minimize memory requirements and permit easy addition of software modules appropriate for new experi-mental methods as they are needed. The programming required may be divided into the two broad classes of a) experiment management and b) data interpretation.

Experiment management software comprises those programs required to:
1. accept operator input of experiment defining parameters such as excitation description, data set volume and time or voltage frequency, etc.
2. generate from the experimental parameters an action list for the experiment control hardware (i.e., "on-the-fly" parameter changes).
3. manage execution of the action list by the control hardware.
4. maintain where possible real time presentations of the progress of the experimental process as it proceeds and respond to operator interaction with that process (e.g., sequencer module, ADC, DAC, etc.).
The ability of the UNC micro-computer to satisfy memory accesses generated by the experiment control hardware while simultaneously maintaining the television display and program execution will permit a great degree of immediacy in the operator's ability to monitor and control his experiment. This property is of particular importance in solid electrode experi-ments where elaborate heuristic "footwork" is often necessary to maintain electrode surface properties.

Planned data interpretation software will extensively exploit the commonality of mathematical treatment often given to electrochemical data acquired through a variety of techniques. Interpretive aids available to the researcher will include various linear and non-linear regression algorithms, simplex fitting of transient responses to theoretical ones generated by finite difference simulation, plus a highly general spectral analysis Fourier package (i.e., for digital filtering, semi-integral type analysis, etc.). Heavy emphasis will be given to the graphic presentation of raw and reduced data with provision for graphic input of reduction parameters.

Electrochemical experiments encompass a wide assortment of techniques. However, they all involve the application of an excitation signal and the measuring of some response to the stimulus. The differences between the various techniques are characterized by the type and time-profile of the excitation, the type and time relationship of the response function to the excitation and the hydrodynamic conditions maintained in the electrochemical cell. Because of the diversity of approaches used in different experimental situations, a universal computer-controlled system is particularly suitable as a general, multipurpose tool in electrochemistry.

The system envisaged would generate the proper excitations, measure the responses and be able to interpret the resulting data for an extremely wide selection of electrochemical techniques. It would also have the capability to perform certain specialty functions indicated in the figure.

A large amount of the appeal of this design results from a very versatile excitation signal source. Waveforms of almost any desired complexity can be generated. These waveforms include steps and the emulation of a ramp function. In addition, a FFT routine available in the spectrum analysis package permits the use of simple or combined sinusoidal excitations. Once the desired signal pattern is chosen (constructed), it may be repeated any number of times.

The excitation signal may be applied to control either current or potential. One of three responses is then measured: potential (for current excitation) or current and/or charge (for potential excitation). By matching the proper signal and response, most classical techniques can be performed.

By using small perturbations in combination with steady state or slowly changing (ramp) signals, the small amplitude class of excitations may be produced. Some of the techniques relying on these are A.C., square wave, triangular and staircase polarography and A.C. chronopotentiometry.

The system is designed to be extremely easy to interact with; thus for simple waveforms, such as the triangular wave, the bounds, sweep direction and a hold function can be controlled as readily as with analog potentiometers and switches. The ability to accurately set up and repeat experiments should be very useful and allow the electrochemist the possibility of increasing data precision.

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