COMPUTERS TEAM UP

WOULDN'T IT BE HELPFUL if you could use a big computer when you need it without tying it up (and incurring the costs) when you don't need it? For some, this problem is solved with a shared-time arrangement.

But if you need some computer capability all of the time and a lot of capability some of the time, the usual shared-time system is not your answer. What you need is a minicomputer with a shared-time big computer.

There is such a thing, and computer technicians call it a hosted-satellite system. One of its best applications is in R&D for analyzing materials and other substances. This work depends on digital computers to control processes and to acquire and analyze data.

There have been countless successful applications of various sizes of computers to all three operations. However, occasions do arise when the data analysis becomes impractical or difficult — although seldom impossible — for persons using such small machines.

One very ubiquitous example is the employment of various non-linear multiple regression techniques in de-convolving spectral lines of all types. The same is true in theoretical curve-fitting and matching.

Other examples are found in areas of automatic indexing of x-ray diffraction patterns, image processing of microprobe data, analysis of particle track data in high energy physics, and, as will be discussed here, reduction of pulsed-nuclear magnetic resonance (NMR) data and electron beam microprobe quantitative analysis.

In such cases, establishment of a hosted-satellite system, that is, direct linkage between your minicomputer and a larger, more-powerful processor, becomes very desirable.

Much time can be spent preparing programs for data acquisition and preliminary analysis for the on-line minicomputer, especially if the applications are changed frequently. In a hosted-satellite environment it becomes particularly convenient to use the facilities of the host for this function, most notably when higher level languages are involved.

Such facilities are desirable even if the satellite is destined to operate in a stand-alone mode after being loaded with its program because the satellite then can be configured primarily for the application without having to include the hardware necessary to support program preparation. For this type of hosted-satellite system to perform effectively, the host should contain the following facilities:

- A macro assembler and a Fortran or PL/1 compiler which produce satellite object code.
- A linkage editor capable of building complete satellite programs plus a utility to format these programs for insertion into the satellite by a variety of physical means (tele-processing links, card and paper tape devices, channels, and so forth).
- A method of effecting conversational interaction between host and satellite either through teleprocessing or direct connection.

Small computers are satellites

In the IBM San Jose Research Laboratory, we are using the hosted-satellite concept to implement project-distributed System/7s connected via high-speed teleprocessing to the laboratory's main computer facility, a System/360 model 195.

The System/7 is a small sensor-based computer with priority interrupt capability. Main storage sizes range from 2 to 16K words of 16-bit length. Direct access disk memory is also available.

Currently, four such machines are installed in our laboratory, servicing the needs of the Analytical Chemistry, E-beam & X-ray Analysis, Mechanical Technology, and Materials Research groups.

These System/7s were configured to permit data acquisition and preliminary data reduction to proceed without the on-line presence of the host and contain 8 to 16K words of main storage with 2.5-million words of auxiliary disk storage. Thus, enough satellite resource exists that experiments can be initiated and run at any time, even if the host happens to be made unavailable by scheduling, maintenance, or malfunction.

The principal role of our host at the present is in the area of System/7 program preparation and data analysis. However, the installation has been designed to permit a more closely coupled and interactive relationship with the host should that become desirable. Linkage to the host takes place through standard telecommunication protocols which were implemented with assistance from IBM's R. Aylsworth.

Special adapters on both host and satellite allow transmission between them at rates of 50,000 bits/sec over in-house twisted pair lines. Hence the host completely can reload the storage of the satellite in four to eight seconds.

The total task of preparing a System/7 program, which includes creating and editing the source text in addition to subsequent assembly, is carried out on the host 360/195 using the time sharing option of Operating System/360.

The user employs a standard IBM 2741 terminal placed in or near his lab for this purpose and is able to have the resulting storage load directed to his particular System/7. Also,

through the terminal, he can initiate background tasks which poll his satellite to commence transfer of acquired data to the host for analysis.

In most cases, the transfer takes only a few seconds so that host processing, either foreground or background can begin immediately. However, a user's data can be buffered in the satellite for an indefinite amount of time prior to conveyance to the host.

In the following, the automation of two widely different types of applications, namely, pulsed-NMR and E-beam analysis, will be discussed in the context of the hosted-satellite system.

The pulsed-NMR operation was designed to depend entirely on the host for program preparation and data analysis. The System/7 satellite is relegated to the task of pure data acquisition, a function it performs in a time-shared manner using a locally developed experimental monitor system for other analytical chemistry instruments (a gas-liquid chromatograph, a gel permeation chromatograph, and a differential scanning calorimeter, among others) in the same laboratory.

This system is called LABS/7, for Laboratory Automation Basic Supervisor, and was written by our Laboratory Automation Systems Group including Aylsworth, G. Hochweller, R. W. Martin, and D. L. Raimondi.

On the other hand, the System/7 satellite attached to the electron beam microprobe has been programed to allow the construction of a simple task-oriented command sequence so that data acquisition mode changes can be made without reverting to the host.

The performance of this function within the satellite was felt necessary in the case of the microprobe because of the large variety of ways the instrument can be used. In contrast, the data acquisition phase of a pulsed-NMR experiment can be defined fairly well. As with the pulsed-NMR, all microprobe data reduction is done on the host.

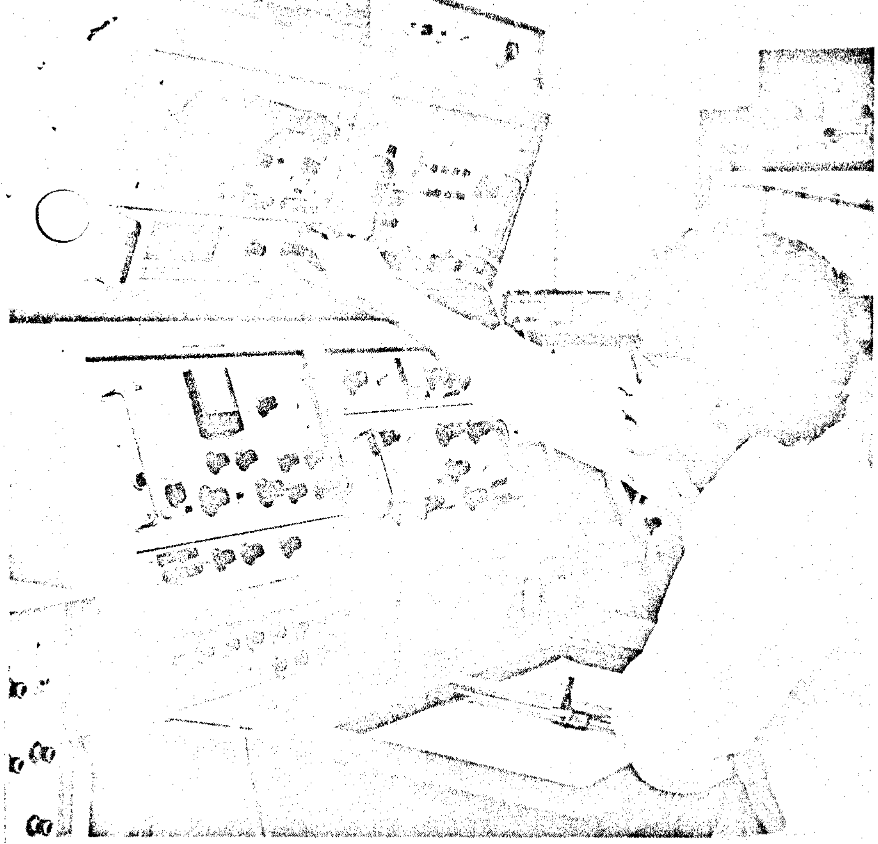
Nuclear Magnetic Resonance provides one of the most powerful methods for determining the structure of organic compounds. The technique derives from the fact that nuclei of certain isotopes possess a spin with resultant angular momentum. Since the nuclei are charged, this angular momentum produces an associated magnetic moment.

When such nuclei are placed in an external magnetic field, their spin axes precess about the field direction in much the same manner that gyroscopes precess in a gravitational field. For the charged nuclei, the precession becomes more rapid as the magnetic field strength is increased.

For example, the simplest of hydrogen nuclei, a single proton, precesses at a frequency of 60 megahertz in a 14 kilogauss field and at 100

ELECTRON-BEAM *microprobe equipment is linked to an IBM System/7 for data acquisition.*

P. M. Grant
T. R. Lusebrink
D. G. Taupin
Computer applications specialists, IBM Research Laboratory.



AN IBM System/7 sensor-based computer gathers data from pulsed NMR spectrometer and feeds it, on command, to host computer.

MHz in a 23 kG field. When a weak radio frequency (rf) magnetic field is applied perpendicular to the static magnetic field at exactly the precession frequency, the spin angular momentum of the nuclei suddenly "flips" to a higher energy state.

The absorption of the rf energy can be detected and recorded as a spectrum. Furthermore, those nuclei surrounded by different molecular environments will have slightly different precession frequencies characteristic of that environment and it is precisely this fact that makes NMR so useful in problems of analytical chemistry.

The two principal modes of operation are continuous wave (CW) and pulsed Fourier transform (FT). In the CW method, the rf field or magnetic field is varied continuously so that the resonance frequency of each nucleus is recorded individually.

In the FT method, the entire range of frequencies is excited with a strong rf pulse and the free induction decay (FID) for all nuclei as a function of time is observed. This data must then be Fourier transformed to obtain the desired absorption spectrum that one obtains directly with CW techniques. From this point, subsequent high resolution analysis of the data from both methods is identical.

Writing in a higher-level language

Most programs of interest to NMR spectroscopists for the analysis of spectra are written in higher level languages, such as Fortran or PL/1, for use on relatively large data processing computers.

Some examples are programs for high resolution spectral analysis, resolution enhancement, calculations of exchange broadened spectra, calculations of various NMR parameters, and so forth. In our system, the original data are transferred, as described above, to the M195 host from the System/7 connected to the spectrometer.

If the data are from an FID experiment, automatic phase adjustment is applied to obtain the desired absorption spectrum. This phase adjustment is necessary because of the time delay between the fall of the rf pulse, when all excited nuclei are in phase, and the beginning of the measurement of the free induction decay at which time phase coherence has been lost.

This delay, in turn, is necessary because of transients induced in the detecting circuitry by the strong rf field. Through a process involving Hilbert transformations of the Fourier transformed raw data, the host is used to correct the phase error.

Currently a 100-MHz NMR spectrometer, operating both in the CW and FT modes, and a gas chromatograph are attached to the System/7. Programs are being written for a differential scanning calorimeter and a light scattering experiment. The latter will be controlled interactively by the satellite.

Three gel permeation chromatographs and a tensile strength tester will be transferred to this System/7 from the current 1800 installation. All data reduction will be done on the host.

MAXOL experimental command language

MAXOL COMMANDS	COMMENTS
MTL SAMPLE, MN-GA-GE	This command labels the run. The sample is the ternary compound MnGaGe (5).
MKV 15	The beam voltage is noted as 15 Kv for later use in data analysis.
MCR LIF	The crystal in this spectrometer is LiF. The satellite uses this to help find peak positions.
MPK MNKA	Initialize to find Mn K-alpha peak by looking up its position in satellite stored tables.
MTC 20	Counting time will be 20 seconds at this peak.
MGO	Start positioning and counting for this peak.
MPK GALA	The rest of the commands do the same as above for Ga L-alpha and Ge K-alpha. Unaltered commands remain in effect until changed.
MGO MPK GEKA MTC 10 MGO	This sequence of commands could be stored in the satellite and reused without reentering. The data acquired by the above sequence would be stored on the satellite disk to await transhipment to the host for analysis and reduction as described earlier.

The only computations, which will be carried out on the satellite, will be time averaging and plot production for a local storage tube display and a general purpose xy recorder.

Probing with an electron beam

Use of the electron beam microprobe (EBM) in quantitative analysis is based on the phenomenon of x-ray fluorescence. When an electron beam of sufficient energy—usually between 1000 and 50,000 volts—impinges on a given material, x-ray photons are emitted.

Their energies are characteristic of the elements making up the specimen but are practically independent of the surrounding chemical environment. This near independence arises from the fact that the fluorescence is produced by transitions involving innermost shells as final states.

It should be clear that the intensity of the fluorescence radiation from any particular element is roughly proportional to its concentration in the specimen under examination as long as beam potential and current are held constant. Thus, the instrument can be used for quantitative analysis of the constituent element concentrations of almost any material.

Structurally, the EBM consists of electron accelerating and focusing optics and x-ray crystal spectrometers for dispersing the resulting fluorescence radiation.

In EBM quantitative analysis, one usually has fairly complete knowledge of the elements contained in the prospective sample. Thus, it is not necessary to scan an entire x-ray spectrum but only to preposition the spectrometer at given characteristic x-ray lines. One then records the fluorescence intensities of these lines with respect to those taken under the same conditions from elemental standards.

Sample is calculated easily

To a first approximation, it can be said that the ratio of the intensities of the x-ray peaks in both sample and standard is proportional to the ratio of concentrations of these elements. Since the concentration in the standard is known, the concentration of a given element in the sample easily can be calculated.

Unfortunately, this approximation is accurate only to a precision of 20%. For more precise estimates of the concentrations, corrections must be applied to the intensity ratios.

The necessity for such corrections arises from several factors, the most important of which are nonabsorption, or backscattering, of some of the incident electrons on the sample; the dependence of the capture probability, or ionization cross-section, on atomic number and beam voltage; re-absorption of emitted x-rays within the sample; secondary fluorescence caused by primary x-rays of shorter wavelength; and background fluorescence.

Algorithms that attempt to correct for these artifacts have been derived, programed, and widely distributed and used. It should be noted, however, that many of the mentioned effects, themselves, depend on element concentration. Therefore, any attempt to compensate for them completely must be iterative in nature.

As is the case with NMR, most of these programs are written in higher level languages and most conveniently are executed on at least a medium-sized computer.

It's all straightforward (relatively)

Automation of the data acquisition and control aspects of an EBM is relatively straightforward. Digitally controlled stepping motors are used to position the spectrometers and move between sample and standard.

Satellite digital I/O features also are employed in setting timers and reading scalers. However, the variety of ways the instrument can be configured to accommodate the diversity of samples encountered renders impractical any attempt to cover all possibilities in one data acquisition and control program.

Thus, it was felt necessary to create a simple command language specific to electron beam microprobe operations whose elements would be executed by a command processor, or interpreter, resident in the satellite System/7. Furthermore, since certain operation sequences invariably will occur more often than others, features were developed permitting the storing of certain command sequences as "programs."

This experimental command language, developed for internal IBM use only, has been named MAXOL, for *M*icroprobe *A*nd *X*-ray *O*perating *L*anguage.

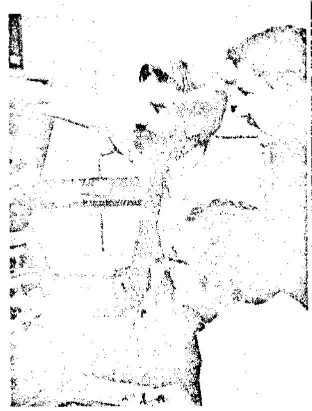
In addition to the EBM, a conventional x-ray powder diffractometer has been connected to the System/7. MAXOL commands have been created to scan through Bragg angles recording the position of the diffraction peaks.

It is planned to send this raw data to the M195 host for line shape refinement, lattice parameter determination, and perhaps complete crystal structure deduction. Also in the process of being instituted are search-match methods using the ASTM file for qualitative analysis.

We feel that the hosted-satellite approach is an optimal one for those laboratories containing a previously-installed general-purpose computer system used primarily for engineering and scientific computations.

This opinion would be particularly reinforced if that system were a time-sharing one and had a history of active use by the laboratory staff. However, we do not deny that alternative implementations of laboratory automation systems well may prove quite attractive.

In other kinds of installation environments where, for whatever reason, access to a central computer facility is not possible or is very difficult, complete stand-alone operation of the instrumentation computers or time-sharing on a medium-sized process control computer may well provide the best solution. ■



THE AUTHORS
Dr. Paul M. Grant, standing, left, has a PhD in applied physics from Harvard. He is responsible for lab automation throughout IBM's San Jose complex.
Dr. T. R. Lusebrink, seated, concentrates in the IBM Research Div., on computers in a scientific environment. His special emphasis is NMR spectroscopy.
Dr. Daniel Taupin is Maitre de Recherches *with CNRS, the principal French national research organization. He is working at IBM, San Jose, as an exchange fellow in laboratory automation.*