Some new developments are changing things for the better: the computer offers the scientist relief from the laboratory grind

To the laboratory scientist the promise of the computer is relief from a growing burden of seemingly endless tabulations and computations that reduce his effectiveness as an investigator. The computer's capacity for accumulating data, plotting graphs and making complex calculations can change the obstacle course of numbers into a clear path of discovery.

The first bright promise of the computer, however, has not been fulfilled overnight. Often the pioneering computer-using scientist found that he was exchanging one form of drudgery for another. Putting the computer to work meant complex programming, interfacing of instrument and computer, of man and machine. Again, precious laboratory hours seemed to be going down the drain.

Two recent developments make the computer more acceptable to the reticent scientist. The first is the small, instrument-oriented digital computer, a relatively low-cost machine with easy-to-use controls, often pre-programmed to do a specific job . . . as in the lunar sample analysis experiment described later. Second is the shared-time computer, which reduces the physical presence of the computer in the lab to nothing more complex than a typewriter-like keyboard. When coupled with packaged programs developed by instrument manufacturers for a specific analytical purpose—as in the simulated distillation article described next—shared-time computer leasing will satisfy increasingly larger numbers of scientists. In both cases, the scientist can capture the advantage of the computer without suffering its complications.

Shared-Time Computer Helps GC Simulate Distillation

A far cry from the alembic used by the 16th century alchemist, the artful glassware used by the modern oil chemist for True Boiling Point (TBP) distillation nevertheless employs the same basic technique: boil and condense. To this day, TBP distillation remains the only accepted way to establish the basic marketing specification of petroleum products . . . and it leaves a lot to be desired. Those who refine petroleum products don't like it because it takes so long: TBP distillation of a wide-boiling distillate can take as long as 100 hours, and the results are useless in controlling the operation of a refinery. Those who buy petroleum products don't like it because the method is not very reproducible, especially as it applies to the initial and final boiling points. Those who perform the distillation don't like it because the procedure itself is a long and boring task.

A group of scientists at HP's Avondale Division have devised a completely automatic method that employs gas chromatography (GC) to simulate distillation and produces boiling point distribution data more precisely and in much less time—about 40 minutes—than TBP distillation. The new method employs the HP 7600A Chromatograph System which is capable of automatic operation from sample measurement to analytical data.

The recipe for simulated distillation with the 7600A is relatively simple. Set the GC for a linear program of 6 to 10°C/minute starting at −20°C, load the sample tray with as many as 36 different calibration and analytical samples, even of widely diverse boiling ranges up to 1000°F . . . and push the *start* button: the rest is automatic.

The 7600A automatically injects the samples and prepares a punched tape record of the GC retention time and area measurements at precise time intervals. Complete sets of programs provided with the 7600A enable any of the principal time-sharing computer services (including the HP 2000A Time-Shared System) to read the punched tape data, determine the initial and final boiling points of each sample, assign boiling temperatures to each data point and print out the analysis report of boiling point distribution of each sample at 1% increments.

No knowledge of computer programming is required by the analyst. At each stage of the computer-performed calculations, the computer asks for the information it requires and the operator answers by typing the requested number or word on the time-share terminal keyboard.

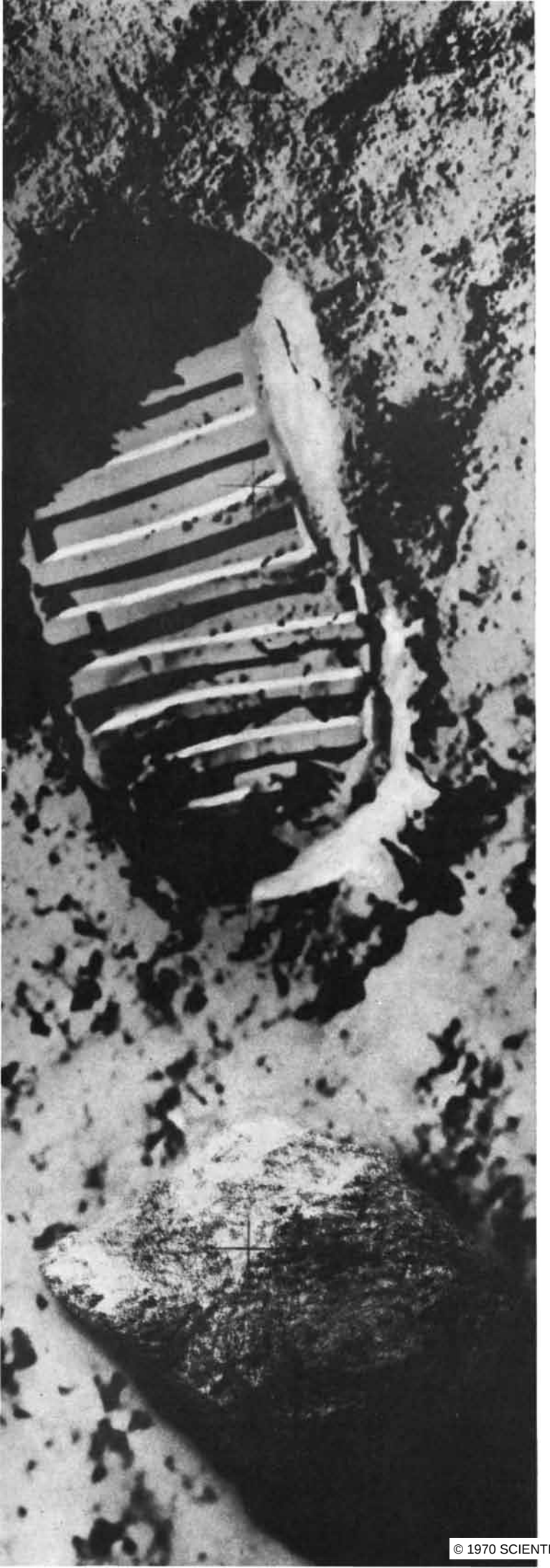
The precision of the 7600A Simulated Distillation method with wide boiling range samples is greater than is possible by any distillation method. Its speed—an average of 40 minutes per sample—completely outclasses distillation methods.

This new automated Simulated Distillation method is examined in much more meaningful detail in Vol. 2, No. 3 of *Analytical Advances*. Request your copy today.

Dedicated Computer Extracts hidden Information from Lunar sample

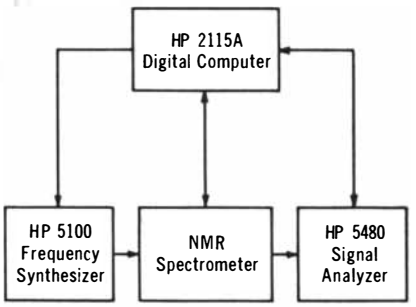
Some of the most respected scientific teams in the U.S. and eight foreign countries are performing analytical investigations on the lunar material returned to earth by the Apollo 11 crew. Among the 100-odd investigations scheduled by NASA, a nuclear magnetic resonance (NMR) analysis will be conducted by a Jet Propulsion Laboratory team headed by Dr. S. L. Manatt. Its goal is to characterize hydrogen nuclei in lunar material and attempt to establish whether any of it can be traced to free or crystalline water molecules presently on the moon's surface. The JPL scientists will also be on the lookout for heavy hydrogen whose presence will allow some conclusions about the history of the moon's surface and about the effect of the solar wind. A study of oxygen-17 may give them important clues about the current chemical environment of the moon (from surface samples) and about the presence of a lunar sea or ocean in the distant past (from core samples).

Present-day commercial NMR spectrometers are capable of accomplishing, unaided, the work assigned to the JPL team with



a creditable degree of success. But when you're analyzing samples that cost about a million dollars a gram to acquire, you're not satisfied with anything short of the best possible performance from your analytical instruments.

In the JPL team's quest for enhancing NMR sensitivity, they devised a system that combines the NMR spectrometer with a frequency synthesizer and signal analyzer under the control of a small digital computer, the HP 2115A, dedicated to this task alone.



The computer-controlled system extracts very weak NMR signals from heavy noise, enhancing instrument sensitivity as much as 100 times. It also performs fast Fourier Transforms of the NMR signal, converting it from time to frequency domain, for a further increase in sensitivity of another order of magnitude.

Here's how it works: the computer digitally sweeps both the frequency synthesizer and signal analyzer through programmed frequencies. Synthesizer output excites the NMR spectrometer which develops noise-covered resonance spikes for each nucleus in the lunar sample; under computer control, the frequency synthesizer also shifts NMR excitation between the resonance and transition frequencies of the nucleus under observation, thereby permitting measurement of relaxation or resonance decay times. The NMR output signal is fed to the signal analyzer which extracts the data from the noise and presents a calibrated display of the average signal at all times. The computer then processes the waveform, converts it from time to frequency domain by Fourier transformation and displays the result immediately in analog as well as digital form. End results of computer-controlled signal averaging and Fourier Transform is to increase spectrometer sensitivity as much as a thousand-fold. (Photo courtesy of NASA.)

Detailed information on HP Signal Analyzers and Computers is available on request. Write to Hewlett-Packard, 1503 Page Mill Road, Palo Alto, California 94304. In Europe: 1217 Meyrin-Geneva, Switzerland.

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