



Computer-Aided Research at Caltech

One of the most exciting developments in the use of the computer is its application in the laboratory

At Caltech today computers are used in almost every facet of scientific research—to perform tedious mathematical calculations, to collate and catalog experimental results, to control laboratory experiments, to gather data, and to analyze the collected information. But the most exciting new development is in the use of computers in the laboratory.

The development of the mini-computer is probably the most significant addition to laboratory instrumentation since the oscilloscope. These machines are now commercially available, and a number of Caltech research groups own mini-computers, which are used to control experiments and to gather and sometimes also analyze data. The “minis” provide great flexibility and remarkable computing capacity at relatively low cost.

A timesharing system like the PDP-10 in Caltech’s Booth Computing Center provides a useful addition to the mini-computer in some cases—and a convenient alternative in others. The expensive high-performance printers, card-readers, volume storage, and other peripherals of the timesharing computer can be “attached” to a laboratory experiment or a mini-computer by telephone line or private cable. And the Booth Computing Center’s powerful IBM 370/158 Batch Processor also becomes accessible to the laboratory via the PDP-10.

On the following pages are just a few Caltech research projects that use the big computers in the Booth Computing Center to directly support their laboratory instrumentation or their mini-computers.

The Gray Group

Harry Gray, professor of chemistry, and his group in Noyes Laboratory use a direct on-line link from their experimental setup to the PDP-10 to help them understand the mechanisms of biological electron transfer reactions.

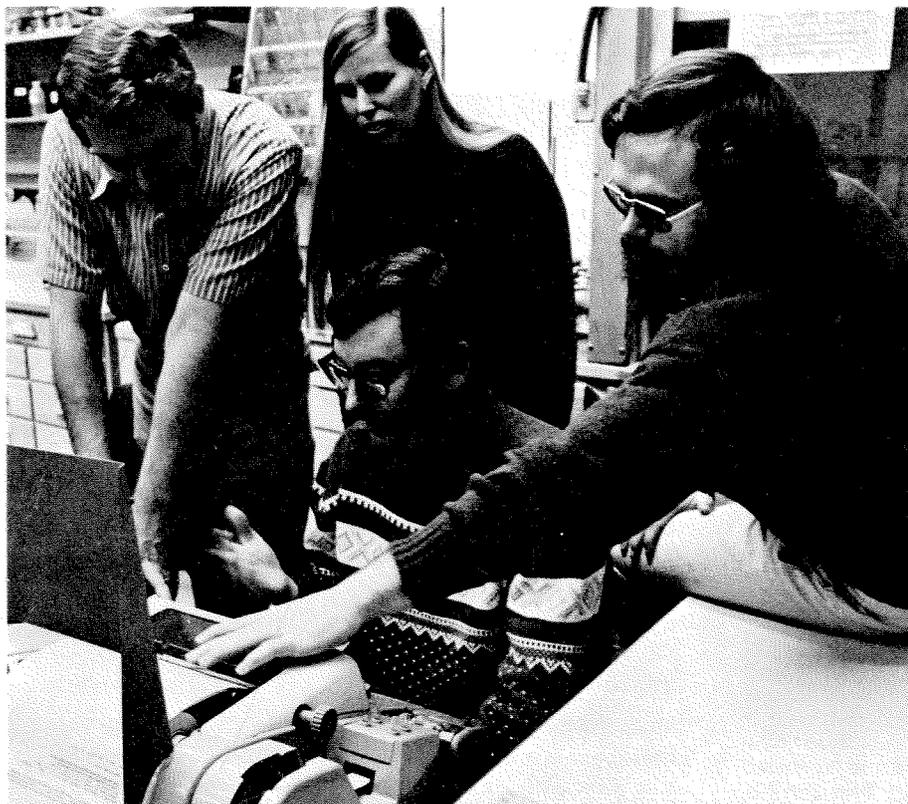
Gray's approach to the question of electron transfer in biology is unique. As an inorganic chemist he is applying standard techniques of inorganic chemistry to a problem in biochemistry. Knowledge of the reactivity of simple metal ions is applied to the understanding of reactions involving more complex species such as the mitochondrial electron transfer protein cytochrome *c*. Cytochrome *c* reacts within a chain of closely coupled redox catalysts involved in the breakdown of carbohydrates by molecular oxygen.

The experiment is designed to measure changes in the amount of light absorbed by a solution of two rapidly mixed species undergoing a reaction. In addition to

cytochrome *c* many other iron- and copper-containing metallo-enzymes are under investigation.

While the study of electron transfer is vitally important, it is also tedious. Rates of absorbance change must be calculated for a wide range of conditions, and the experiment must be performed repeatedly for each set of solutions. Before the advent of the computer in Gray's laboratory, the decay curves of these solutions were constructed by manually plotting one point after another, adjusting the results, and drawing a new graph. Now the PDP-10 collects the information directly from a data storage unit attached to the spectrophotometer recording the absorbance changes, does the necessary calculations, and automatically prints an adjusted plot on the laboratory console.

The Gray group is now able to handle a great deal more data at a much faster pace. And, while storage requirements once limited the speed of the reactions that were studied to tenths of a second, the group is now analyzing reactions as short as a thousandth of a second.



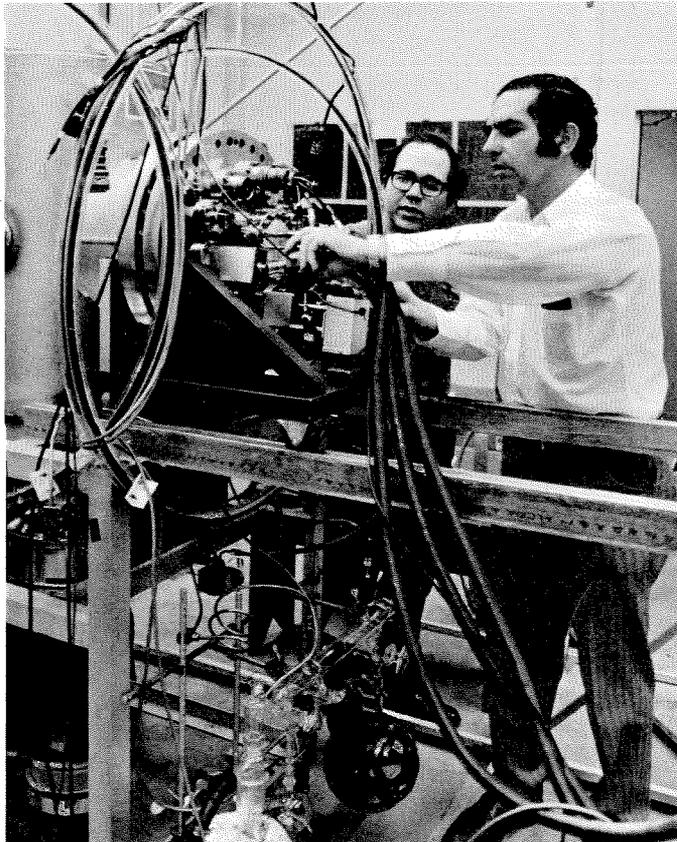
The console in Harry Gray's electron transfer laboratory is receiving reaction results calculated by the PDP-10 in Booth. With Gray are research fellows Bob Holwerda and Leslie Hodges, and graduate student Jim McArdle.

Derek Fender and Eye Movements

Derek Fender, professor of biology and applied science, has a different approach to computerization in his laboratory. In his studies of why and how the eye moves as it does, he uses a mini-computer both by itself and as an intermediary with the PDP-10.

In experiments on what causes the eye to focus on an object first detected by peripheral (side) vision, Fender uses a PDP-11 mini-computer to monitor a subject's eye movements. Graphs of this movement are kept on a regular basis. The subjects must quickly discriminate between nearly identical targets, separated by distances proportional to the level of visual sharpness being measured. The graphs show that in every case decisions are related to a very jerky motion of the eye called a saccade.

Fender's current experiments deal with the way the brain-eye visual system discriminates between objects of different texture. A random number generator in the 158 in Booth produces cards containing two distinct arrays of dots, each with a unique design. The subject's



Graduate student Don Mintz and Aron Kuppermann study the fundamental electronic structure of molecules with this variable-angle photoelectron spectrometer, which is directed by a PDP-8e mini-computer connected to Booth's PDP-10.

task is to decide where the boundary lies. The responses are recorded by Fender's mini and then passed on to the 158, which analyzes the data and relays back a new set of dots.

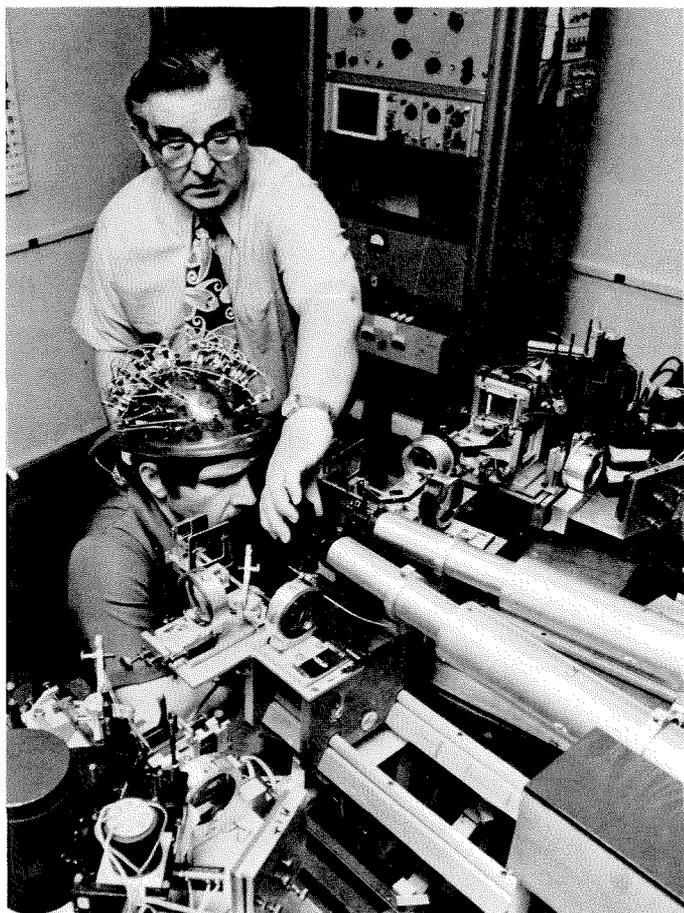
The problem posed is: What are the criteria for distinguishing textures between collections of dots of varying visual texture? Fender and the computer are working on it.

Kuppermann Research

With the assistance of a PDP-8e mini-computer and the PDP-10 in Booth, Aron Kuppermann, professor of chemical physics, is studying the fundamental electronic structure of molecules. He does this by shooting photons at the molecules, then measuring the energy of the ejected electrons over a range of detection angles.

Although the experiment is relatively simple, handling the data is not so easy. Hundreds of runs of the experiment are necessary to pick out the real signals from background, extraneous signals, or noise. Automation is almost mandatory, especially in the data reduction processes.

The principal apparatus used in this work is a variable-angle photoelectron spectrometer. The mini-computer functions as a link with this instrument. It receives and stores the already digitized data and issues control com-



The apparatus Derek Fender is adjusting is used to work out the mapping of connections between the subject's retina and brain. It fixes an image on the retina (one that does not move, even if the subject moves), and the resultant activity in the brain is monitored by a special helmet, worn here by graduate student Tom Santoro.

mands back to the spectrometer. The computer automatically scans a range of energies as the situation demands and also changes the angle of detection. A direct line with the PDP-10 is used to develop programs for the PDP-8e.

Dreyer, Hood, and Antibodies

William Dreyer, professor of biology, and Leroy Hood, associate professor of biology, in separate but similar research projects, are trying to find out exactly how cells synthesize antibodies.

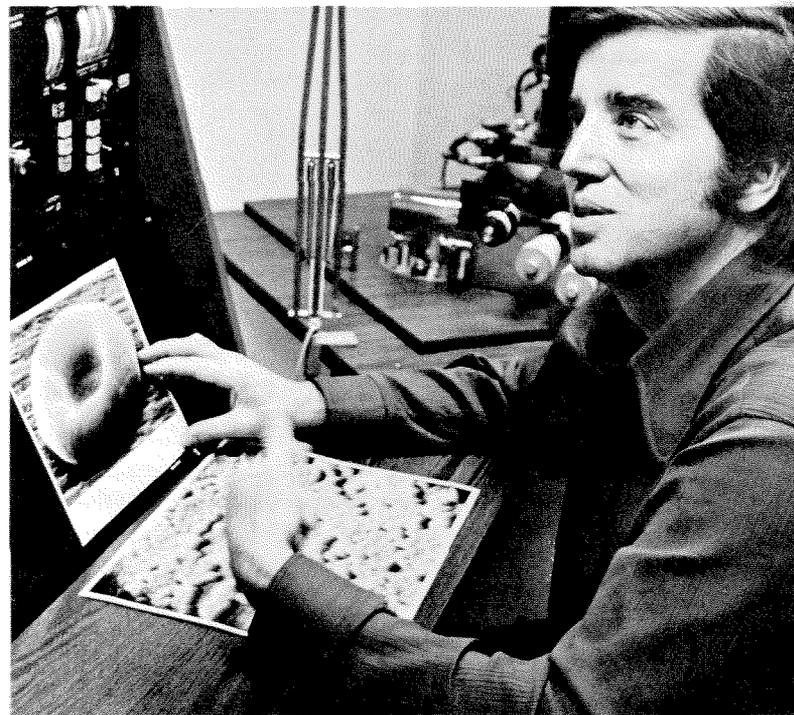
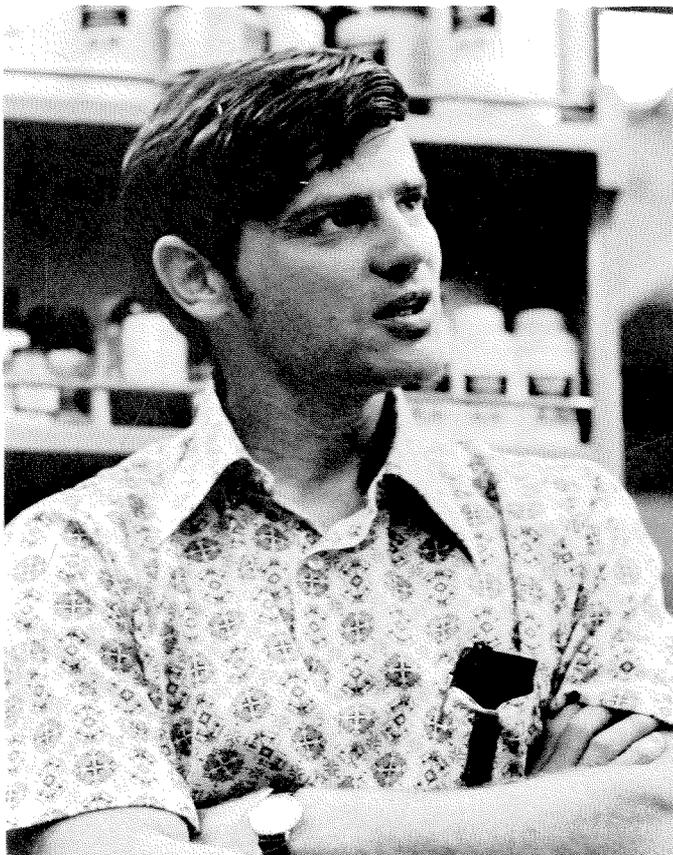
To understand how antibodies are created and how they attack disease organisms requires a complete understanding of the molecules themselves. But there are at least a million different kinds of antibody molecules. And each molecule is an extremely complex protein chain which must be perfectly made to accomplish its mission of annihilation. The phenomenal ordering process in the protein chains is analogous to perfect spelling: not only must each letter be correct, but it must appear in the proper place as well.

To simplify the problem, Hood and his group have concentrated on a special class of antibody proteins, the immunoglobulins, which are specifically responsible for providing immunity to diseases. The experiments of this

group are directed toward determining the sequence and relative quantities of the amino acids that make up these proteins. An amino acid analyzer measures proteins as they are degraded in sequence by chemically separating off one acid at a time. Each run on the analyzer corresponds to a particular amino acid. An understanding of the entire chain involves comparing series of analyses.

The large number of molecules that are studied by Hood's group requires an automated system. Hood records the data with a PDP-8 mini-computer. These are stored on a magnetic tape and played into the PDP-10, where they are sifted and arranged into meaningful information. The results from each run are displayed either numerically or graphically by the computer.

Dreyer is now developing an automated mass spectrometer to do essentially the same research. In his experiments, data will be produced at a much faster rate, and the PDP-10 will be used to control and record the data until industry comes out with a mini-computer designed to operate the mass spectrometer.



Biologists Leroy Hood and William Dreyer, in separate but similar research projects, are trying to find out exactly how cells synthesize antibodies.

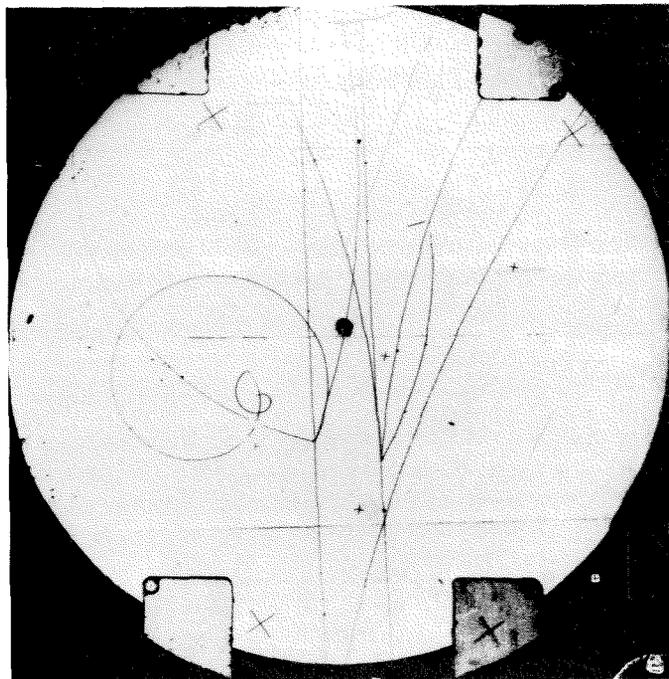
POLLY

A group of high-energy physicists are using the PDP-10 to control a film-measuring machine called POLLY. Their research is aimed at understanding the strongest force known, the one that binds the atomic nucleus together. POLLY's Caltech contingent, including Alex Dzierba, Charles Peck, Ricardo Gomez, and Alexander Firestone, is analyzing the results of experiments done two years ago at the Stanford Linear Accelerator Center.

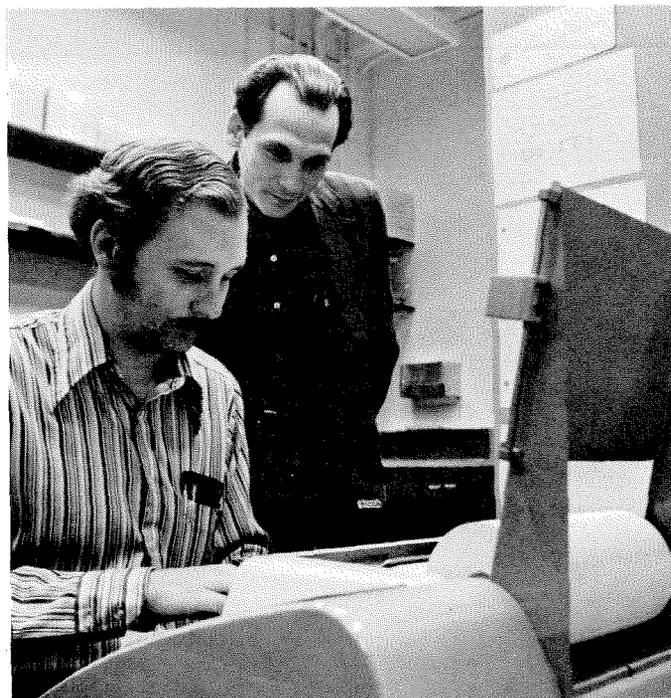
The goal of the research is to measure the diffraction dissociation of protons by pions. To do this, high-energy pions bombard protons in a bubble chamber. This device contains a highly compressed volume of liquid hydrogen. Just before the pions enter, a large piston retracts, allowing the hydrogen to expand and to become superheated in the process. The paths of the particles then show up as tracks of bubbles in the chamber.

During the experiment, three cameras, at different angles, simultaneously photograph the bubble chamber events on 70-millimeter film. POLLY's job is to measure the coordinates of bubbles on this film. From this information, the momenta of all the particles involved in a collision can be determined. The Caltech group, and their collaborators at UC Berkeley and Stanford, are now deciphering the information from more than a million pictures.

Each track must be measured rapidly and precisely. To satisfy this requirement, POLLY uses a complex computer-operated instrumentation system—in this case a PDP-11 mini-computer linked to Booth's PDP-10. An operator initiates the measurement of a track by pointing to it on an optical display of the picture. The computers then drive the spot on a precision cathode ray tube (CRT) so that its image falls on the film where the operator indicated. The CRT spot then executes a series of short sweeps, and, by observing where light is transmitted through the film, POLLY makes a precise measurement of one point on the track. The computers are programmed to make intelligent searches for other track points, so that, from a single, relatively crude, manual measurement, precise coordinates are quickly obtained along its full length. This is repeated for all tracks in an event, and finally, the computer's image of its track analysis is displayed on a terminal screen and compared with the original picture for accuracy and completeness.



An example of the type of picture being measured by POLLY, showing the materialization of particles from the energy of the incident pion. The pion beam enters from the bottom. Here, two of the incident pions have collided with protons in the bubble chamber and, in the process, two new charged particles have been created. In the event on the left, one of the outgoing pions has undergone radioactive decay, and the track shows an apparent sharp change in direction. By measuring the coordinates of points on these tracks with POLLY and the PDP-10, it is possible to determine the momentum of each particle. By studying many such events, physicists hope to learn more about the mysterious inner workings of the strongest interactions in nature.



Tom Garrard (PhD '72), staff scientist, and Edward Stone study some of the features of the program that controls communication between their mini-computer and the PDP-10.



Searching for relatively rare oxygen nuclei in cosmic rays, graduate student Solomon Vidor checks out a tape from the SRL library.

Browsing in this library of 7,000 tapes is economically feasible only with the aid of mini-computers and the PDP-10.

The communications link between the two computers is such that the PDP-10 issues commands for the operations, the PDP-11 performs them, and then returns data to the PDP-10. The track measurements are eventually sent to UC Berkeley where three-dimensional stereo views are reconstructed from the data, and the momentum of each track deduced.

Space Radiation Laboratory

Caltech's Space Radiation Lab (SRL) is using the PDP-10 to display processed information collected over the past decade in numerous satellite and balloon-borne experiments.

SRL's current studies are based on information from five NASA-supported satellites orbiting the earth within half the distance of the moon. These high-flying laboratories were designed by physicists Ed Stone and Rochus Vogt to analyze the composition of solar and galactic cosmic rays.

The satellite data are received and stored on magnetic tapes by the Goddard Space Flight Center—and the tapes are eventually added to SRL's enormous tape library housed in the Downs-Lauritsen laboratories at Caltech. It is the volume of information on these tapes that prompted a link with the PDP-10.

Plans now call for the creation of a condensed, problem-oriented data library available for student use. For example, except during periods of solar flare activity the detection rate of oxygen nuclei in cosmic rays is very low. With the current setup, dozens of tapes must be sorted, and scattered data gathered, before calculations of any kind can be done. The condensed tapes will have all the necessary information in one place.

The link between SRL's mini-computer and the PDP-10 facilitates the display of information from this library.

—Gary Prohaska, '73