Meetings

Computer Assisted Chemical Research Design

In the past decade, computer technology and design and the development of low-cost "minicomputers" and "integrated circuitry" have advanced at an almost unbelievable rate. Thus, computers and computer-based instrumentation now readily available to the chemist are revolutionizing research in chemistry. The applications of computers in the areas of computation, information storage and retrieval, data acquisition and reduction, simulation, and instrumentation (on-line data processing and experimental control or optimization, or both, in real time) has opened up a new dimension in research.

Although chemists are beginning to work with these new techniques and tools and are also developing new methods and instrumentation, we have found, in general, that, on an individual basis, we have only a limited awareness of the new developments in the area of computer uses in chemistry. Thus, the joint Japan–United States seminar, which was held in Honolulu, 2 to 6 July 1973, was designed to bring together representatives working in many different aspects of computer uses so that we could find out what new developments have been made, to learn how these new developments could be used in our own specific areas of research, and to consider areas of future developments and needs.

An overview of the various applications of computers in chemical research and the basic aims of the seminar were given by S. Fujiwara (University of Tokyo). A brief introductory discussion of how the minicomputer (used in real-time mode in experiments) enables the chemist to carry out new types of studies that were not previously possible because of time, manpower, and instrumental capabilities was presented by H. B. Mark, Jr. (University of Cincinnati). The application to time-resolved multiple component phosphorescence decay studies was given as an example. The rest of the papers were then divided into two broad categories: (i) real-time applications of minicomputers in experiments and instrumentation and (ii) uses of the large computer systems in data processing and information retrieval.

With respect to real-time applications, C. N. Reilley (University of North Carolina) discussed the importance of making a detailed specification of the tasks to be performed and constraints imposed by the nature and types of experiments to be carried out before designing the computer system for real-time data acquisition and reduction and experimental control (automation). He described how the central minicomputer system which serves approximately 25 varied instruments and types of experiments in the chemistry department at the University of North Carolina was designed and constructed. S. P. Perone (Purdue University) then showed how on-line minicomputers can be used in the feedback loop of the experiment itself for automatic optimization of experimental parameters during the actual course of the experiment and how it can also be made to interact with the experimenter. S. R. Crouch (Michigan State University) discussed the automation of stopped flow kinetic measurements and a multielement atomic fluorescence instrument. D. E. Smith (Northwestern University), S. Fujiwara (Tokyo University), C. N. Reilley (University of North Carolina), and S. Minami (Osaka University) showed how fast Fourier techniques can be used advantageously in electrochemical kinetic and spectroscopy studies. The complex design problems (and their ultimate solutions) in the construction of a computer-controlled multiband microscanning sensor were explained by T. Kunii (Information Science Laboratories, University of Tokyo) and I. Sawamura (Olympus Optical Company Ltd., Tokyo). K. Konishi (Kao Soap Co., Ltd., Wakayoma City) and H. Kaneyuki (Mitsui Petrochemical Ind., Ltd., Iwakuni) described two industrial automated analytical quality control systems.

Discussing complex data treatment and information services, T. Sakai (Faculty of Engineering, Kyoto University) reported on an extensive computer network system for information processing. Although the examples given—speech wave analysis, line drawings and photographs, and character coding—are not directly related to chemical problems, they were stimulating because these techniques could be applied to chemical research. The immediate needs for computerization of the immense amount of information in the chemical literature are realized by all chemists. The capabilities and limitations of information storage-retrieval systems were discussed by M. Williams (Coordinated Science Laboratory, University of Illinois) and T. Yamamoto (Computer Center, University of Tokyo). P. C. Jurs (Pennsylvania State University) showed how pattern recognition techniques can be applied to chemical data interpretation and S. Sasaki (Miyogi Kyoiku University) described a computer program for automated chemical structure analysis from nuclear magnetic resonance and infrared spectra. An information retrieval system capable of estimating thermodynamic properties of organic compound from data available on similar compounds, component functional groups, and the like, was described by Y. Yoneda (Faculty of Engineering, University of Tokyo). M. Hatori (Department of Electrical Engineering, University of Tokyo) described data communication systems in Japan.

In the session on future development, C. N. Reilley discussed low-cost easily tailored "microcomputers" which might be the solution to the establishment of practical, hierarchical, computerized data acquisition and analysis systems to service many laboratories simultaneously. Considerable interest was generated by the possibility of having a microcomputer which would cost about $1500 and be capable of acting as an intelligent terminal or as a stand-alone dedicated computer (or both) for real-time experimental uses. B. Crouthamel (Data General Corporation, El Segundo, California) discussed developments in hardware and software to be expected from minicomputer manufacturers. Earlier in the week, each participant had been asked to submit a list of topics related to future areas of development and need in computer uses in chemical research. These suggestions fell into the following categories: hardware, man-machine interactions, system organization, standardization, software, information exchange, applications, library, education, and possible future symposia. All the points in each category were discussed briefly.

All the participants expressed a need for expert technical assistance in computer hardware and software design in the chemical laboratory and thought that chemistry departments could profit by the addition of a full-time computer scientist. Everyone reported, however, that their individual administrations were not enthusiastic about creating such positions in chemistry departments and interaction and communication with personnel in other departments and computer service groups was difficult.

The seminar was sponsored by the National Science Foundation and the Japan Society for Promotion of Science under the Joint United States–Japan Cooperative Science Program and was organized by H. B. Mark, Jr., and S. Fujiwara. The proceedings will be published by the University of Tokyo Press.

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Geodynamics Symposium in Mexico

The symposium on geodynamics held in Mexico City 20 through 24 June was the first of its kind to be convened in Latin America. Though shortage of funding prevented the attendance of as many colleagues from other Latin American countries as we would have liked to see, the meeting was truly continental in scope.

Three main topics were examined: (i) regional problems of the Americas, (ii) driving mechanisms of sea-floor spreading, and (iii) deep-seated mechanisms of geophysical fields. The final session consisted of a field trip into the Cuernavaca Valley.

The sessions on regional problems, which was chaired by Fernando de Almeida of the University of São Paulo, got off to a brisk start with a well-illustrated full-length lecture by Charles L. Drake, who reviewed the subject of geodynamics—past, present, and future. Talks were delivered by Ernesto López Ramos (PEMEX) on the paleogeography of Mexico, by James N. Brune *et al.* on the Gulf of California, by Roger A. Stacey on western Canada, by Roland von Huene on the Alaskan continental margin, by LaVerne D. Kulm on the Oregon-Washington continental margin, by Peter Vail (Esso Research) on the Central American continental margin, and by Cecilia Bellizzia on Northern Venezuela.

Among the results contributed in these sessions were the preliminary data obtained by Brune on the Colima earthquake of 30 January 1973 and the impressive seismic profiles of the Middle America Trench by Vail, who supplied convincing evidence for accretion of the continental slope.

David C. Tozer led a session on driving mechanisms, and he presented a paper in which he attempted to derive a physical concept of a plate. Like Tozer's discussion, J. Weertman's presentation on the mechanics of ridges and mantle plumes was especially full of fresh ideas.

George P. Woollard was chairman of the final session. In the first talk Yoshio Fukao (Nagoya) offered seismological evidence for down-dip tension rather than bending in the shallow part of subduction zones. George G. Shor *et al.* contributed recent results from the Cocos Plate; Luis del Castillo *et al.* summarized the Mexican gravity data, Martin Halpern discussed plate tectonics of southern South America and recent age determinations; Donald Hussong *et al.* showed their recent work off the coast of Peru, and Woollard closed the meeting with what amounted to a keynote address on the joys and disappointments of heat flow, gravity, and other measurements to decode the structure of the crust and mantle under the Pacific Basin.

Round-table discussions took place throughout the meeting. I remember at one of these Mauricio de la Fuente spoke on the Colorado River Delta, J. Negendank on the mineralogy of lavas in the Valley of Mexico, Rafael Rodríguez on tectonic regionalization of Mexico, Roger N. Anderson on the "cold spot" under the Guatemala Basin, and T. Matumoto on aftershocks of the Managua earthquake.

The Sunday field trip included climbing the Tepozteco, a steep volcanic cliff overlooking the village of Tepoztlán. About a hundred participants, with members of their families, undertook the strenuous climb, and nearly all made it to the Aztec pyramid at the top. The exotic geology and the physical effort made this a memorable adventure.

The Mexico Symposium on Geodynamics was programmed as part of the AAAS/CONACYT Conference, and was jointly sponsored by the Inter-Union Commission on Geodynamics and the Mexican National Committee on Geodynamics.

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Forthcoming Events

December

9–13. American Soc. of **Hospital Pharmacists**, 8th, New Orleans, La. (J. A. Oddis, ASHP, 4630 Montgomery Ave., Bethesda, Md. 20014)

10–12. **Sensing of Environmental Pollutants**, 2nd conf., American Inst. of Aeronautics and Astronautics and Inst. of Electrical and Electronics Engineers, Washington, D.C. (AIAA, 1290 Avenue of the Americas, New York 10019)

10–14. American Soc. of **Agricultural Engineers**, Chicago, Ill. (J. L. Butt, ASAE, P.O. Box 229, St. Joseph, Mich. 49085)

10–14. American Geophysical Union, Section on **Hydrology**, San Francisco, Calif. (R. Lee, Div. of Forestry, 337 Percival Hall, West Virginia Univ., Morgantown 26506)

11–14. International Symp. on **Biomembranes**, Madurai, India. (J. Jayaraman, ISB, Dept. of Biological Sciences, Madurai Univ., Madurai 625021)

12–16. American **Psychoanalytic** Assoc., New York, N.Y. (M. A. Berezin, 90 Forest Ave., West Newton, Mass. 02165)

17–19. Conference on **Computers in Spectroscopy**, Soc. for Analytical Chemistry and Inst. of Physics, London, England. (Meetings Officer, IP, 47 Belgrave Sq., London, SW1X 8QX)

17–21. Association of **Engineers and Architects in Israel**, 3rd world congr., Tel-Aviv. (AEAI, Engineers Inst., 200 Dizengoff Str., POB 3082, Tel-Aviv)

17–21. **Marine Waste Disposal**, 2nd intern. congr., Assoc. Nazionale di Ingegneria Sanitaria, San Remo, Italy. (Istituto di Ingegneria Sanitaria del Politecnico di Milano, Segreteria per 1 Convegni Intern., Piazza Leonardo da Vinci, 32 Milano, Italy)

17–23. International Assoc. for **Medical Research and Cultural Exchange**, Yaounde, Cameroun. (IAMR, 4, rue de Seze, 75 Paris 9e, France)

26–30. Society for the **History of Technology**, San Francisco, Calif. (M. Kranzberg, Dept. of Social Sciences, Georgia Inst. of Technology, Atlanta 30332)