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COMPUTING & SYSTEMS TECHNOLOGY DIVISION
OF THE
AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

NEWSLETTER MIDYEAR 1978

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COMPUTERIZED ATLANTA 1978 MEETING

T. I. Peterson, IBM, Armonk

We've talked about it many times, but attendees witnessed it at the 84th National Meeting in Atlanta, February 26 - March 1, 1978. What was it? Well, it may be the Year of the Horse by the Chinese calendar, but this year also saw the introduction of computerized registration. And that's only one facet of how computerized methods assisted in the Atlanta 1978 Meeting. Because the author, who was also MPC (Meeting Program Chairman) for the meeting, chose to use a computerized textual data base in developing the program.

Computerized Registration

First, let's look at how computerized registration was handled. As far as registrants were concerned (those who were not preregistered), they moved from one station (where the information from their registration cards was transcribed, fees collected, and receipt given) to a second station (where their badges were generated).

This was done through the use of a minicomputer for the first step and an intelligent terminal-plotter lash-up for the second step.

The result? An alphanumeric data base was created from which listings of registrants were produced instead of the old "Cardex" system (and up-to-date at all times, at that). Also produced were summary statistics indicating the number of registrants by various types, for the numerous events, and with this, the income derived (again, always up-to-date and available).

The response to the method? Nothing but accolades: from registrants, since queued lines were a thing of the past; from Headquarters and the Meeting Arrangements Comm., since they knew exactly the status of meeting attendance, events, etc., at any point in time.

Any who provided this service? Betty Reece, who heads a company less than two years old, known as Convention Management Systems (Based in Atlanta). And would you believe that she's gone through two generations of equipment with upgrades in that short period of time -- first with IBM and then with WANG equipment?

Computerized Textual Data Base

Not too surprising, then, is the fact that as MPC for Atlanta 1978, the author chose to relegate the mechanics of developing program copy to a computerized textual data base.

From the outset, the embryonic copy took shape, was edited, augmented, and "cut-and-pasted," until it reached the status of the final program copy delivered to Headquarters for printing.

This approach provided two invaluable assets -- control and communication -- control, because the MPC could readily review and monitor the meeting in whatever detail necessary; and communication, because there was a two-way link established to the MPC from all the various contributors, and from the MPC in the form of monthly printouts to all the contributors and others within the Institute.

As a result, everyone involved in the meeting had an up-to-date and accurate document which formed the basis for that all-pervasive and vital man-to-man communication. All appeared pleased, since there was so little confusion resulting from this approach.

(As might be expected, the author did use IBM equipment and an IBM textual application package. But, Verle Schrodt, MPC for the Miami 1978 Meeting is using similar techniques on his own equipment with his own application package).

"C-Cubed" Committee

As one consequence of these demonstrations of the utility of computerized methods, CAST created at Atlanta 1978 an ad hoc committee to advise the Institute in such areas. Dubbed the CCC (for Computer-aided Control and Communication) Committee on Administrative Information, and this "C-Cubed" Committee consists of three members: Ted Peterson (IBM), Mike Tayyabkhan (Mobil) and Ted Leininger (duPont).

This Committee will keep you informed of how computers are being considered to assist the Institute in executing its functions. As "Van" Van Antwerpen has said, "We led the way by computerizing the Directory." Now, with such techniques, the Institute can continue to lead the way in becoming more responsive.

Naturally, the "C-Cubed" Committee welcomes your suggestions (please direct your comments to any member).

ANNOUNCEMENT OF CAST DIVISION LUNCH & MEETING

The executive committee of the CAST Division will meet in Philadelphia, PA on Monday, June 5 from 1:30 to 5:00 P.M. in Temple B Room at the Philadelphia Hilton Hotel on Civic Center Boulevard and 34th St. Division members are invited to attend. The meeting will be preceded by an informal luncheon for members of the division to be held at 12:15 P.M. in the Penn Room. The menu will be supreme of chilled fruit, broiled chopped sirloin steak, apple streussel and beverage. The cost is $9.30 including taxes and gratuity. Send your reservation and check, payable to "Hilton Hotel", to Sigmund J. Lawrence, 10 Yorkshire Drive, East Windsor, NJ 08520. Lunch reservations must be received by May 26.

SYMPOSIUM ON COMPUTERS IN PROCESS DESIGN AND CONTROL

Two sessions will be held at the Miami meeting, November 12-16, 1978. Warren Seider of the University of Pennsylvania is Chairman. Larry McCane of Monsanto is Co-chairman.

The conference will focus on new, innovative techniques of direct interest and application to the process industries. The session will not be devoted to conventional process simulators nor to computer control installations. The hopeful topics will be:

- Advances in process simulation
- Uncertainty and reliability analysis
- Process optimization
- Process synthesis
- Multivariable and adaptive process control
- Simulation and control of batch processes
- Application of engineering data bases
- Computer graphics in process design and control

NEWS OF CAST MEETING IN ATLANTA

A bare quorum enabled the executive committee of CAST to transact business at the Atlanta meeting on Monday, February 27th at the Peachtree Plaza Hotel.

There are 335 members (as of 2/27/78).

A division information booth will be established at the Institute meetings. The appointment of CAST Board Chairmen was accomplished and these names appear at the beginning of this newsletter.

The bylaws provide for the membership to establish sections via petition. Therefore, if you are interested, contact the secretary, Bob Fisher.

A "CAST Guide" for the exposition tours will be prepared by Mac Clarke and distributed in the registration area at the Philadelphia meeting.

Ted Peterson reported on the rise of computers for the registration procedure initiated at this meeting. See Ted's write-up elsewhere in this newsletter. CAST, through an ad hoc committee chaired by Ted, will work with the National Programming Committee to provide assistance with computer techniques and applications.

Henceforth, because of cost considerations, newsletters will be sent to paid members only. Once a year, the newsletter could be sent to selected non-members as part of our promotion literature. An extra 200 copies of this issue will be available for distribution at the Philadelphia meeting.

A logo (masthead design) was selected. It appears at the top of the first page of this issue.

This is the tenth year for CACHE. Dave Himmelblau is the new chairman. The FLOWTRAN workbook is available.

Status of ASPEN: FLOWTRAN is implemented on the MIT computer. FORTRAN is to be used exclusively.

(Cont. on Page 7)

OFFLINE - REVIEWS

In this part of the newsletter we will attempt to briefly review or to bring to your attention items, articles, papers, magazines, books, or whatever strikes our fancy and which we feel might be of interest to chemical engineers involved with computing. No attempt will be made at restricting these reviews to only newly published items, since we are constantly discovering ideas, techniques, and concepts that are new to us as we explore various areas of computing and will be of interest to you also.

For this issue we will look at one new book recently published and also survey some of the new magazines now being published as a result of the growth of personal computing. First for the books:

> Numerical Methods for Partial Differential Equations
> William F. Ames; Academic Press, NY
> Second Edition (1977) $16.50

Numerical Methods is a thorough updating of a book that has become a standard in the field of numerical techniques. Divided into six parts: Fundamentals, Parabolic Equations, Elliptic equations, Hyperbolic Equations, Special Topics, and finally, Weighted Residuals and Finite Elements. The first four parts are similar to the first edition except for the addition of recent work, more applications, and references. In the fifth part numerical fluid dynamics is looked at in fair detail, while the sixth part is new to this edition. This section gives a limited introduction to the method of weighted residuals, briefly describes orthogonal collocation with no example and essentially says that the finite element method exists! These last areas are gaining much recognition as powerful tools useful for many chemical engineering problems.

Numerical Methods is definitely a basic reference, filled with information and pointers as to where to find additional information. Well worthy of purchasing, though be warned, it is not a cookbook in that there is not a single line of code or a flowchart in the entire book.

The Method of Weighted Residuals and Variational Principles by B. A. Finlayson, Academic Press, (1972), details how useful these techniques including orthogonal collocation can be in solving chemical engineering problems, such as the boundary value P.D.E's to O.D.E's which then can be handled by the new powerful integrators such as Gear or Episode.

In the last two years, what was anticipated to happen in the 1980's has already happened; that is, the availability and reduced cost of new computer hardware which allows the purchase of personal computers by individuals. Concurrent with this availability many magazines have been started which are designed for the personal computer hobbyist. These journals can be of value to the chemical engineer involved with computing since they are written on several different levels and cover topics such as new hardware, computer concepts, programming techniques, numerical methods, simulation, games, etc.

Briefly surveyed are:

> Creative Computing P.O. Box 789-M, Morristown, NJ 07960
> Bimonthly, $8.00 per year.
>
> Kilobaud Peterborough, NH 03458,
> Monthly $15.00 per year.
>
> Byte Subscriptions P.O. Box 590, Martinsville, NJ 08386,
> Monthly, $15.00 per year.
>
> Personal Computing 1050 Commonwealth Avenue, Boston, MA 02215,
> Monthly $14.00 per year
>
> Ram, Computer Applications for living, Route 97, Hampton, CT 06247,
> Monthly, $15.00 per year.
>
> Popular Computing Box 272, Calabasas, CA 91302,
> Monthly, $17.50 per year.

Creative Computing has been around for four years and has been considered to be the number one source of computer games. But wait, this magazine is aimed at a much

broader area. For example, in the January - February 1978 issue, good articles include: File Structures (Part 2); Topics in Logic: Turing Machines, World 2 - A version of Forrester's World Model; Grammar as a programming language; A new Fast Sorting Algorithm; How to Write a Computer Simulation. In addition there are several other articles that present mathematical and logic problems, excellent book reviews, and of course - games. This book is interesting and also fun, highly recommended.

Kilobaud is a magazine concerned with small computers which attempts to be understandable to beginners and interesting for experts. The March 1978 issue covers hardware extensively as well as software. Articles include:

Hardware Program Relocation
Number Crunching Time
Programmed Instruction Made Easy:
Tiny Pilot
Temperature Sensing
Backup Techniques
IP Programming for the Altair Disks

Kilobaud is apparently aimed at helping a user evaluate hardware, assemble a system, and to a lesser extent use the system. Thus articles that might be of interest are not of the level of Creative even though they consist of a lot of meat at times.

Byte, subtitled the small systems journal, does not try to be everything for everybody. Again, this publication looks at both hardware and software, often with issues having several articles of a common theme. The March 1978 issue for instance has two articles on computers and music: A Two Computer Music System - on hardware; The Micro-computer and the Pipe Organ - on software. In addition, other articles include: Controlling the Real World - A Basic Introduction to Process Control with Micro-processors; The Brains of Men and Machines: Part 3, How the Brain Analyzes Input. In addition this publication offers ample information on what is available, new developments, etc.

Personal Computing has a good visual impact but has not yet found what type of audience should be the target. Articles in the FEB. 78 issue include: Big memories for Micros; Technology and the Times: Computer Graphics (An Article in general terms that focuses on special effects in the movie Star Wars); Building your Basic Robot. This magazine has some interesting articles that are easy to read but have no real content. Previous issues varied widely in level of articles.

Rom is a magazine difficult to categorize. In the January 1978 issue articles include a long description of a new language - TLC which is designed as a real world language aimed so that a TLC program should read like a "job description" for a computer written in English. This article is fascinating and it is apparent that the writer has a lot of good ideas. However, near the end of the article, we find that this language does not yet have a compiler and translation to machine code is to be done by you. Other articles include a long extract from Weizenbaum's book Computer Power and Human Reason; Mirco-computers Help the Deaf; Codebreaking; and to top it off: Snythetic Skin for Your Robot and How To Make It.

Popular Computing is quite different. Quite thin, 20 pages at $2.50 per copy, $17.50 per year. This publication which has less text than our last news letter, is nevertheless quite fascinating. It is a publication designed for those who are interested in computing for its own sake. This journal consists of problems in mathematics and logic to consider. In the Dec. '77 issue are included: A problem on Sorting Which is a Contest; a short extract from Computers and the Social Environment, Wiley (1975) on How to Produce Garbage (excellent commentary on common computer problems); Exploring Random Behaviour; Counterfeiting (an article that leads to a description of ciphers); An Exercise in Logic; and a few other problems to solve.

My favorites of the above publications are:

Creative Computing - Since it touches on a lot of areas which enlighten me in the field of computer science and also because I like games. Supplement this with BYTE to see what is happening in this new and growing area of personal computing - Hardware, applications, and some software. If you want to be challenged try Popular

Computing. The problems are similar in some ways to Martin Gardnor's column in Scientic American, but do not get into the areas of Topology, etc. that his do. Don't eliminate the other publications though. Drop into one of the many new personal computing shops that are appearing every where and browse through these publications. Who knows, some new idea will appear!

For a future issue of Offline - Reviews we would like to compare a top 5 or 10 list of books on numerical analysis. We welcome your nominees along with comments. Send these to me:

Joe Zemaitis
c/o OLI Systems, Inc.
15 James Street
Morristown, NJ 07960

CENTER FOR INFORMATION AND NUMERICAL DATA ANALYSIS AND SYNTHESIS (CINDAS)

For the past 15 years this Center, stationed at Purdue University, has operated for the Dept. of Defense a National Center known as the "Thermophysical and Electronics Properties Information Analysis Center" (TEPIAC), to serve the needs of the DOD and its contractors for reliable numerical data covering thermophysical, electronic, electrical, magnetic and optical properties of various materials.

If you would like to get on the mailing list for the bimonthly Newsletter, Annual Report, special notices, etc. write to:

TEPIAC/CINDAS
2595 Yeager Road
West Lafayette, Ind. 47906

Provide your organization name and address, your title and organizational function and your areas of interest.

FUTURE CAST MEETINGS

1978		
	Philadelphia	June 4 - 8
	Miami	November 12 - 16
1979		
	Houston	April 1 - 5
	Boston	August 19 - 22
	San Francisco	November 25 - 29

BYTES AND PICOS (BITS AND PIECES)

This issue is being sent only to paid-up members of the CAST Division. The reason is economics.

At the Philadelphia meeting, look for the computer tour guide at the registration desk.

The 1978 Joint Automatic Control Conference (JACC) will be held at the Civic Center in Philadelphia, October 18-20, 1978. The theme of the Conference is "Control Theory Meets the Real World of Applications", and appropriately, this meeting is being held in conjunction with the ISA/78 International Conference and Exhibits, which consists of a technical program and 70,000 sq. ft. of control hardware exhibits.

News Item - Huge black hole found in Washington, D.C. Source is believed to be centered in government bureaucracy.

Don't forget the gala CAST Division dinner at the Miami meeting.

NEWS OF CAST MEETING IN ATLANTA

(Cont. from Page 4)

Nominating Committee - If you have any suggestions, contact Charles Ware.

Awards Committee - Warren Seider is looking for a chairman. Charles Ware volunteered to do the contracting.

COMPUTATIONAL ARCHITECTURES IN PROCESS SIMULATION - Feature article by Rudy Motard

For over ten years industrial process engineers have been using computers for the steady state simulation of mass and energy balances in complete chemical processes. Today, close to one-third of the new chemical engineering graduates have been exposed to sophisticated process simulation programs. Several thousand practicing engineers have been active users of the medium at some time in their careers.

By far the most common computational architecture for simulation programs is the sequential modular method. This method is the easiest to implement and understand while generating stable computational procedures. Each unit model has a clear identification with a physical operation and its input and output data are the descriptions of the process streams in the plant. Output streams from a unit model are computed from its input streams and a minimum of given design parameters.

Despite the maturity and acceptance acquired by the sequential modular method, a growing list of architectural options are becoming available from the collective research of academics and industrial engineers. They are:

1. Sequential Modular
2. Equation Solvers
3. Sequential Modular with Successive Linearization
4. Linear
5. Quasi-Linear
6. Simultaneous Modular
7. Decoupled
8. Data-based

The newest and most exciting developments, with the greatest promise of high computational efficiency are the last four in the list. All methods except the first have been developed to overcome some of the drawbacks of the sequential modular method. They are intended to improve the speed of convergence in recycle computations, to reduce the amount of computation when unit output constraints are imposed, i.e. design specifications, to accelerate the search for optimal design parameters and operating conditions and to integrate process simulation into a coherent process engineering environment.

Equation solvers have had a long history, but have met with limited success because of the difficulty of constructing stable solution procedures for large systems of non-linear equations. They will probably never achieve widespread use when the user performs the tedious task of preparing equations for the model. Nevertheless, when coupled with process compilers that automatically generate equations from a modular description of a process they are enjoying renewed vitality. In particular, if the choice of dependent and independent variables in the compilation is controllable by the user to direct the information flow in the model, then there could be some incentive to use such systems in critical applications. Thus, the user may wish to compute input streams from specified output streams for some units in the plant or to calculate the design parameters which match specified input streams to specified output streams at other units in the system.

Successive linearization and linear models attempt to achieve the benefits of the simultaneous solution of system models and their constraint equa-

tions in a minimum number of steps. The motivation is that the system mass and energy balances are linear between the unit models. Non-linear interactions occur only within the units. They are the result of coupling between the mass and energy transformations, chemical reactions or, compositional effects on thermodyanmic properties. Successive linearization is a valid approach to convergence acceleration in itself, but it is doubtful if it provides a substantial advantage over a convergence accelerator applied to suitably selected tear variables as one finds in a modern sequential modular system. Linear models on the other hand are quite useful in evaluating the sensitivity of process designs to inaccurate data or to overdesign specifications and thus have an intrinsic value beyond mere computational speed; a speed which is obtained perhaps at the expense of considerable simplifications.

Quasi-linear systems extend the concept of linearization to whatever depth is necessary within the unit models and their physical property estimation equations to provide a more accurate and efficient solution procedure. Mass and energy coupling and compositional effects on mixture properties are reduced to linear relationships along with the intrinsically linear system balances. The resulting model requires iterative solution, but the convergence rate should approach that of a super-linear acceleration procedure like quasi-Newton. When coupled with process compilation, which allows a modular process description, and sparse matrix methods which speed up the repeated linear solution procedures, these systems provide the most efficient steady state simulators in existence today. Earlier versions could only handle non-reacting systems, but they have recently been extended to include reactors as well.

Simultaneous modular systems do not rely on linearization methods. Instead, this architecture is designed to overcome the multiple nesting of iteration procedures which is so prevalent in sequential modular systems. For instance, a flash calculation in a sequential modular system is always converged at the unit model level before the system recycle convergence is attempted. This "loops-within-loops" approach is very time consuming. To improve the situation a simultaneous modular system attempts to put all iteration variables both at the unit level and system level on one common level to be accelerated simultaneously. The process description is modular, but each unit model is designed to execute only one pass through it's various levels of iteration. Internal iteration variables are transmitted to the system convergence routine to be accelerated along with the system level tear variables in global fashion. Substantial improvements in speed have been reported; on the order of five to ten times faster execution than the sequential modular method.

Decoupled systems offer an interesting variation suitable for interfacing to an optimization procedure. Process streams in the model are not automatically linked between their sources and destinations, but rather they acquire two identities, one as an input stream and a second as an output stream. The units of a process model may be decomposed at the subsystem level where each subsystem is a collection of units. In the latter case the decoupling is between subsystems rather than between units. Optimization of the separate subsystems independently using a dual formulation of the optimization objective yields a lower bound on the overall objective function, say annual cost, of the system and a set of sensitivity measures. The user may then choose to redefine the structure of the most sensitive subsystems

to effect a maximum improvement in the objective function. When the entire procedure converges, the source and destination versions of the coupling streams have been matched by virtue of a final run using the primal formulation of the problem.

Data-based systems may have some of the properties of decoupled systems, but the primary emphasis is on the integrity of the project data and on the management of multiple data banks. A conventional view of process simulation is that the program itself would reside somewhat permanently in the computer and the data, in the form of punched cards or a disk-resident I/O file, would be "passed by" the program. In a data-based system, the data for a specific project are given equal priority with the program. The program segments which comprise the simulation or design program may be "passed-by" the data in an incremental fashion or in a total analysis of the plant. The data reside in a data base management system within the computer. Access to and updating of the data is carefully controlled. The object of controlled access is to make the collective efforts of a project or design team manageable. Each engineer may read data for any part of the project, but may only change or update those data for which he has been given authority by the project manager. Extensive data banks of physical property data, catalogs of design data, etc. can be made accessible to the design programs. Recoding of input or output data between various stages of design is eliminated since all design activities access a common data base. Various design standards and error checking techniques may be imposed on the data as they are passed through the data management system interface at the several stages of design analysis. Multiple representations of a process plant may be maintained for the manifold purpose of design and some automatic recasting of representations may be visualized, e.g. automatic translation of parts of a process flow diagram into parts of a piping and instrumentation diagram.

COMPUTING & SYSTEMS TECHNOLOGY DIVISION

AIChE

Membership Application.

I wish to join the newly formed C&ST Division of AIChE. My dues payment of $3.00 is enclosed.

NAME_____

ADDRESS_____

_____

_____

EMPLOYER (IF NOT IN ADDRESS)

_____

My two primary areas of professional interest are:

_____

_____

(NOTE: Sections devoted to specific professional areas of interest will be formed within the division.)

I am willing to work on a Division Committee:

( )	Programming	( )	Special Interest Sections
( )	Publications	( )	Awards
( )	Membership	( )	Other

Complete the above form. Staple your check (made out to CAST Division, AIChE) to it, fold and mail it to the membership chairman:

R. E. Harris
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Cleveland, Ohio 44115