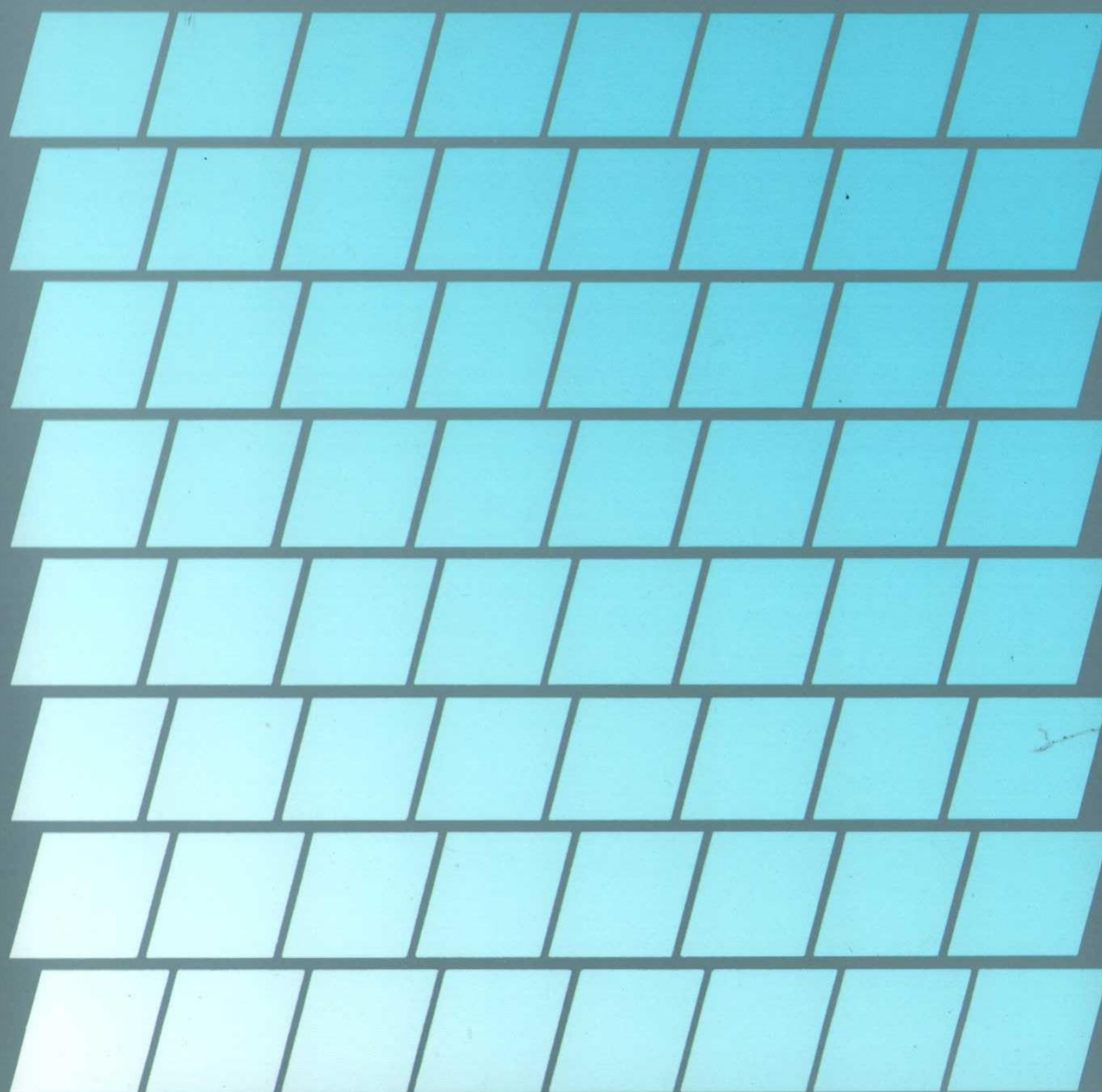


Computing Technology

for the benefit of Industry



HARWELL

Computing Technology

for the benefit of Industry



HARWELL

Computing Technology

The key to Harwell's success is that we work in close collaboration with our customers. This ensures that they benefit from the practical application of new technology. As part of Harwell's wide range of skills and facilities, we offer advanced computing services and develop computing products for individual customers and for more general use. In the following pages we describe computing facilities and software which are routinely used by a large number of organisations.

Working with Industry

Our Computer Science and Systems Division provides advanced computing services, specially designed software and develops new computing techniques.

Major areas of expertise are:

*Supercomputing services
Interactive graphics
Applications software
Mathematical modelling and numerical techniques
Information systems
Advanced computing and knowledge based systems
Scheduling and planning
Decisions support systems
Software engineering*

Harwell is the major laboratory of the UK Atomic Energy Authority. Our scientists and engineers rely extensively on advanced computer facilities and applications software packages.

Supercomputing Services

Powerful computing facilities are essential for the work of the United Kingdom Atomic Energy Authority. The Harwell Computing Centre is one of the largest and most advanced computing centres specialising in scientific and engineering applications in Europe. Supercomputing facilities, the development of software and new computing techniques play a significant role in Harwell's work. Bureau services, software and consultancy are supplied to industrial, government and academic organisations.

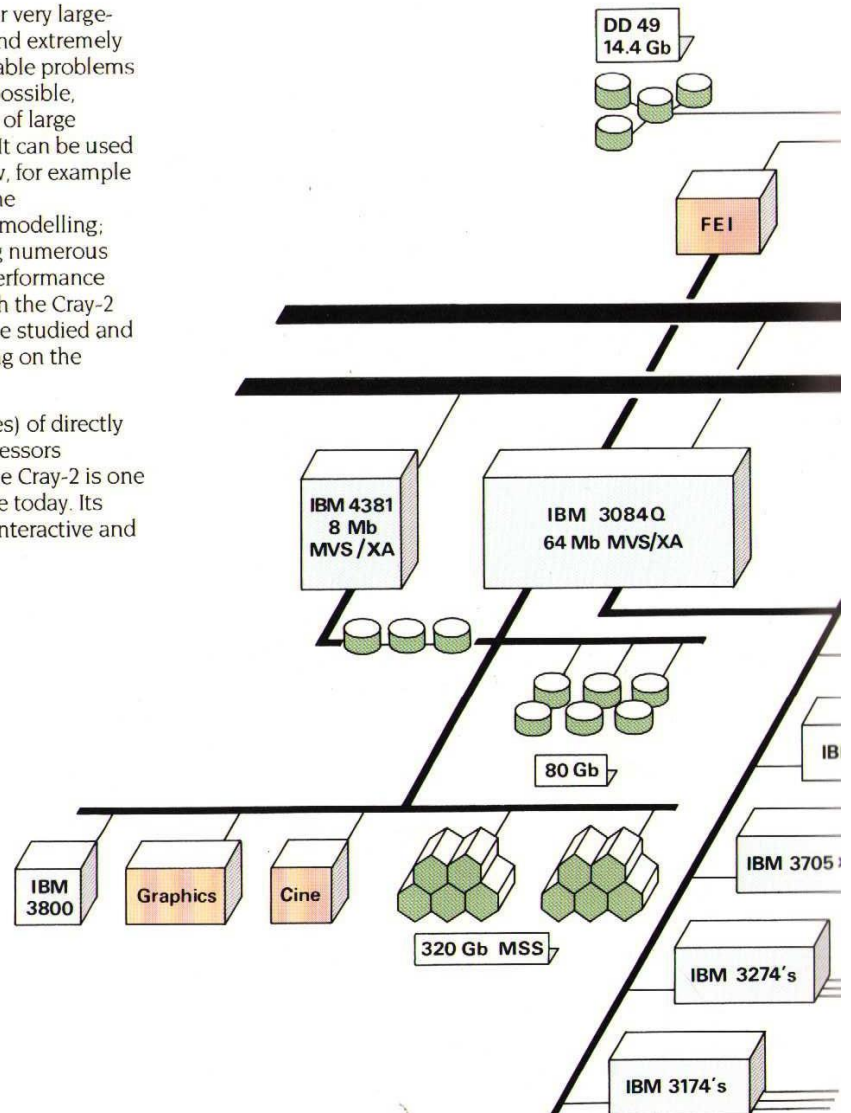
The IBM 3084Q operating under MVS/XA is the main 'workhorse' within the Centre. It is used for routine scientific calculations, scientific data processing, computer aided design, management information and database applications. It also provides the central file store to supplement the Cray disc storage, allows access to the Cray-2 and supplies supporting services such as high quality printing and plotting. This computer has 64 Megabytes of main memory and 400 Gigabytes of on-line storage.

Harwell Computing Centre

The computers installed at the Centre include a Cray-2, an IBM 3084Q and a VAX cluster. All of these are interconnected by means of a 50 Megabits/sec Hyperchannel local area network.

The Cray-2 supercomputer is designed for very large-scale calculations. Its massive memory and extremely fast processors enable previously intractable problems to be solved. New applications are now possible, including three dimensional simulations of large complex systems on a production basis. It can be used to advance research in the way fluids flow, for example in nuclear reactors or heat exchangers; the development of new materials; financial modelling; computational chemistry; and for solving numerous engineering problems. The use of high performance graphics workstations in conjunction with the Cray-2 enables the progress of applications to be studied and controlled whilst the program is executing on the supercomputer.

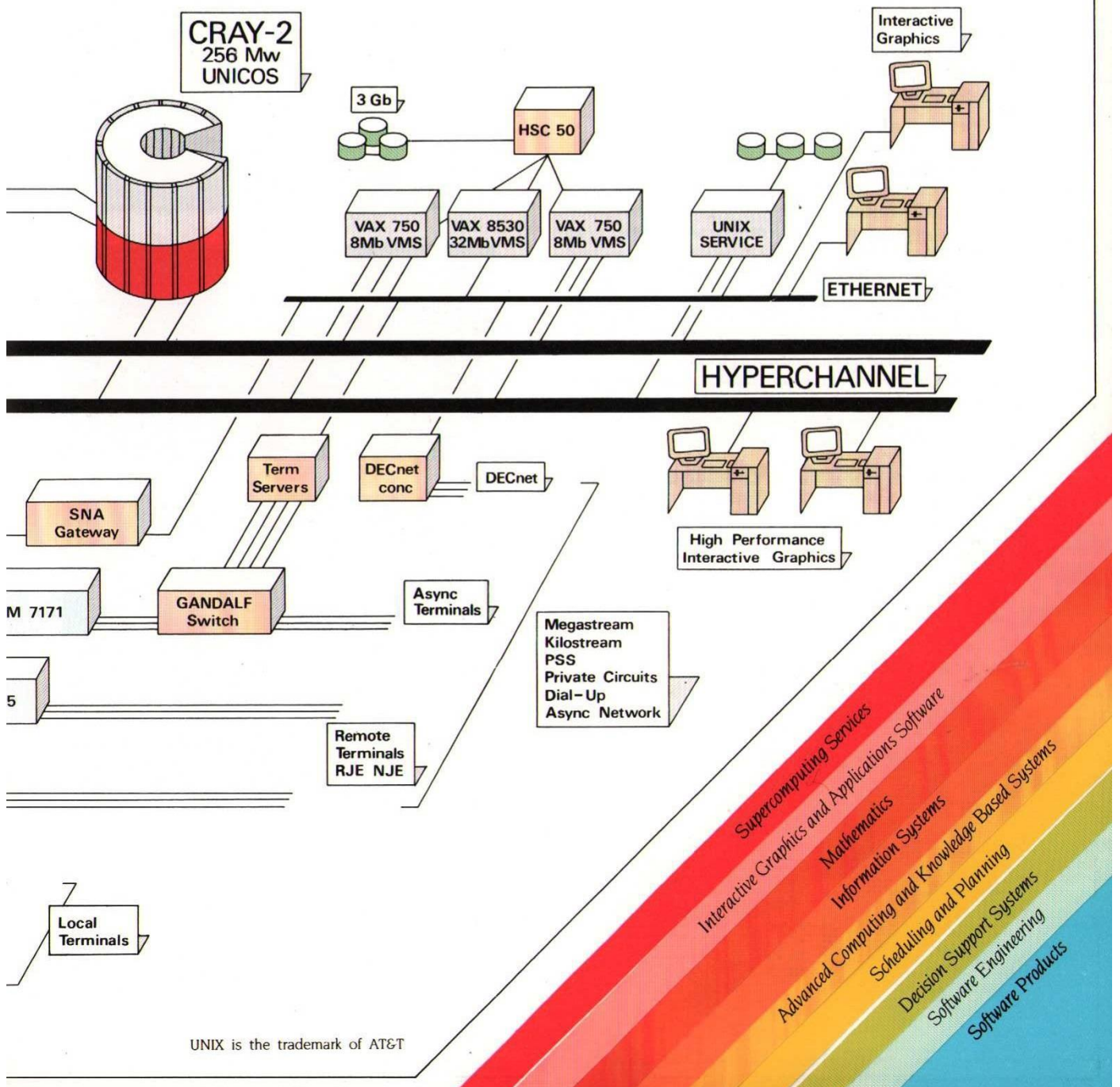
With 256 Mega (64 bit) words (2 Gigabytes) of directly addressable main memory and four processors operating with a 4.1 nanosecond clock the Cray-2 is one of the most powerful computers available today. Its UNICOS operating system provides full interactive and batch facilities.



The DEC/VAX cluster includes a VAX 8530 and a number of smaller VAX computers. This system is an alternative access route to the Cray-2, as well as supplying production VMS services.

A number of communications protocols are supported including SNA, DECnet and TCP/IP. The service can be accessed from local and remote locations with line speeds up to 2 Megabits/sec. Telecommunications links include: Megastream, Kilostream, PSS and dial-up.

A very wide range of applications and systems software are available. The Computing Centre is run to commercial bureau standards throughout the year by a highly skilled and professional staff, who are dedicated to the provision of first rate leading edge computing services.



UNIX is the trademark of AT&T

Interactive Graphics

To complement the Supercomputing Services, the Harwell Computing Centre has advanced graphics facilities and is adding a number of popular third party software packages to its already large portfolio.

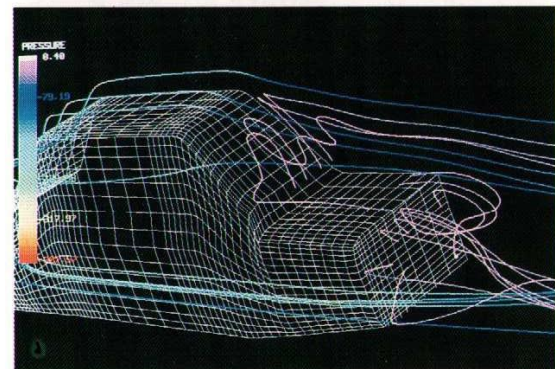
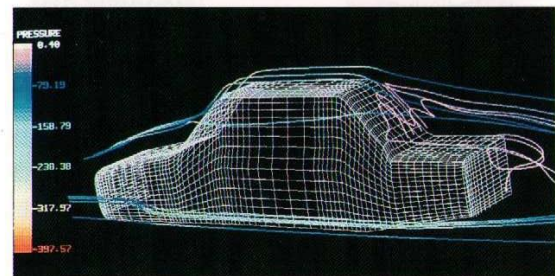
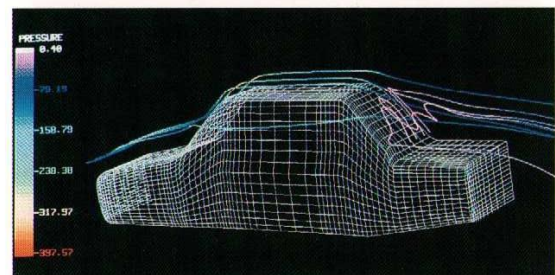
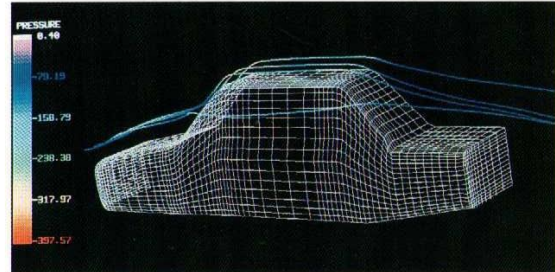
Advanced Graphics

Advanced graphical display systems are essential for one to be able to comprehend the results of massive calculations and complex simulations. This is particularly true with some of the applications now being run on the Cray-2 supercomputer, which may produce tens or even hundreds of thousands of data values.

The Computing Centre supports a number of modern graphics packages together with a range of output devices for producing plots, slides and film.

For the more advanced applications, static two dimensional representations are inadequate and have been supplemented by the use of high performance graphics workstations. These devices permit the result of complex calculations and simulations to be viewed in four dimensions – a 3D rotatable representation with colour providing the fourth dimension. By connecting these UNIX based computing engines directly to the Cray-2 the engineer can in effect “see” the progress and results of programs executing on the supercomputer, with recordings for permanent record. This formidable combination of vast processing power coupled with multi-dimensional graphics displays is opening up the new field of computational science, that allows the engineer to go beyond observations and theory, and actually simulate natural phenomena.

Some of the applications now exploiting these new technologies are molecular dynamics, fluid dynamics, structural analysis and geophysics, through to the biomolecular patterns that underlie life itself.



Prediction of the flow over a vehicle using FLOW3D.

Applications Software

A number of software packages have been installed on the Cray2 computer for fluid dynamics calculations, nuclear safety, stress analysis, graphics and mathematical techniques. These include:

ABAQUS

A general purpose finite element program for advanced engineering applications, with special emphasis on non-linear problems.

DYNA3D

An explicit 3-d finite element program for analysing the large deformation dynamic response of inelastic solids.

FAM

A suite of programs for field analysis modelling for the discretizing techniques FEM, BEM and FDM. The modules comprise interfacing from CAD, pre-processing and interfaces to the main FEM packages like ABAQUS, ANSYS and NASTRAN. FAM offers the engineer a unified interface to ease the use of alternative analysis programs. The open architecture allows for interfacing to special purpose programs.

Harwell FLOW3D

A general purpose code for the simulation of laminar and turbulent flow and heat transfer in and around complex geometries.

GHOST

Graphics package.

GINO

Graphics package.

Harwell Subroutine Library

Nearly 400 subroutines for numerical and mathematical analyses, particularly strong for the solution of large scale problems.

MOVIE BYU

A general purpose computer graphics system.

NAG Library

A collection of over 500 routines for mathematical and statistical analysis.

PHOENICS

A general purpose code for simulating fluid flow, heat transfer, chemical reaction and multi-phase phenomena.

RELAP

For predicting the behaviour of PWRs and BWRs subjected to postulated transients, such as loss of coolant, pump failure, power excursions etc.

TRAC

For best estimate analysis of loss-of-coolant accidents and other transients in light-water reactors.

UNCLE

A finite element package which provides general transient and steady-state heat transfer facilities, including the exchange of radiation between arbitrary surfaces, natural and forced convection, latent heat and variable material properties. It analyses thermal stress, pipe and framework stress. UNCLE includes an extremely powerful mesh generator for the other modules or for any other finite element code.

The suppliers/originators of the applications software packages are:

ABAQUS	- Hibbit, Karlsson & Sorenson Inc. 35, South Angel St., Providence RI 02906 USA Tel: (401) 861 0820
DYNA3D	- Argonne National Laboratory, National Energy Software Centre, 9700 South Cass Ave., Argonne, IL 60439, USA Tel: (312) 972 7250
FAM	- FECS Ltd. Oakington, Cambridge CB4 5HA, England Tel: 022 - 023 - 7111
Harwell FLOW3D	- Harwell Laboratory, UKAEA Tel: 0235 - 432865
GHOST	- Culham Laboratory, UKAEA, Abingdon, England. Tel: 0235 - 21840
GINO	- Computer Aided Design Centre, Madingley Rd., Cambridge CB2 0HB, England. Tel: 0223 63125
Harwell Subroutine Library	- Harwell Laboratory, UKAEA Tel: 0235 - 432865
MOVIE BYU	- Engineering Computer Graphics Laboratory, 368 - CB - Brigham Young University, Provo, Utah 84602, USA. Tel: (801) 378 2812
NAG Library	- Numerical Algorithms Group Ltd., Mayfield House, 256 Banbury Rd., Oxford OX2 7DE, England. Tel: 0865 511245
PHOENICS	- CHAM Ltd., 40 High St., Wimbledon, London SW19 5AU, England. Tel: 01 - 947 - 7651
RELAP	- EG & G Idaho, Inc., PO Box 1625, Idaho Falls, ID 83415, USA. Tel: (208) 526 - 9461
TRAC	- Group O - 9, Los Alamos National Laboratory, Mail Stop K 553, Los Alamos, NM 87545, USA. Tel: (505) 667 - 2021
UNCLE	- Risley Technical Services, UKAEA, Warrington WA3 6AT, England. Tel: 0925 31244

Interactive Graphics and Applications Software
 Mathematics
 Information Systems
 Advanced Computing and Knowledge Based Systems
 Scheduling and Planning
 Decision Support Systems
 Software Engineering
 Software Products

Mathematics

Complex problems arise in many industrial or chemical processes, and the best solution is not always immediately apparent. Trial and error approaches are time-consuming and expensive, and produce uncertain results. However, by the construction of a computer model, the physical situation can be represented in a mathematical form, and a range of options can be simulated to determine the optimum conditions under which a system should be operated to achieve its objectives.

Several software packages which apply mathematical methods to solve complicated real life problems have been developed at Harwell. Applications in which these modelling techniques have been used include:

- fluid (liquid and gas) flow in systems
- chemical reaction kinetics
- oil and gas reservoir modelling
- reactor coolant models
- flow in furnaces and combustion engines.

For the development of these packages, extensive use has been made of the subroutines in the Harwell Subroutine Library. The Library has a high standard of reliability and a worldwide reputation as a source of good numerical codes.

Major projects in this area include:

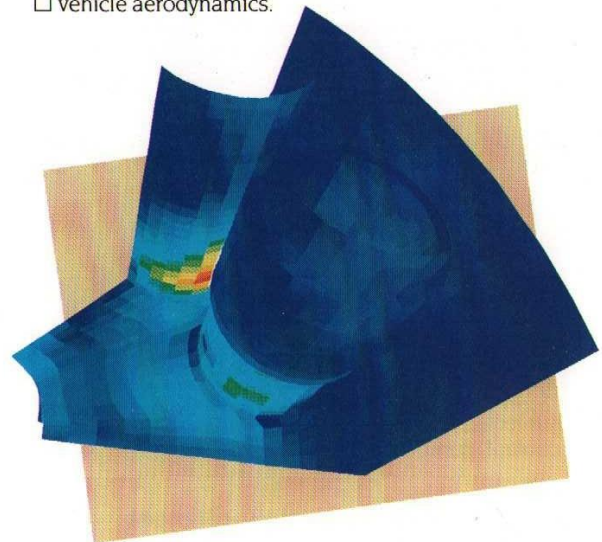
Flow Modelling

Harwell FLOW3D is a general purpose code for the simulation of laminar and turbulent flow, and heat transfer, in two and three dimensions. It is being developed by an interdisciplinary team both as an efficient and reliable tool for engineers to use on practical simulations and also as a vehicle for research into new solution techniques and physical models. The code is able to deal with compressible and incompressible flows in complex geometries using body fitted co-ordinates. Methods for predicting two phase flow are being included.

The numerical methods are based upon standard finite difference (or finite volume) techniques for obtaining discrete equations which conserve mass, momentum and energy in individual 'brick-like' control volumes. The software and the physical models are being subjected to extensive validation.

Some applications are:

- complex flows in furnaces and engines (in combination with combustion models);
- measurement/characterisation of detailed flow patterns in heat exchangers;
- reactor coolant circuit modelling
- the study of crystallization and separation;
- discharge of cooling water from power stations;
- modelling smoke and fire growth in buildings;
- studies of fluidised beds;
- vehicle aerodynamics.



FLOW3D is user orientated with three self contained modules, a front end for problem specification, a solution module and an output/graphics module.



Tony Stone Worldwide

Reaction Kinetics and Transport Simulation

FACSIMILE is a rugged and efficient suite of closely related computer programs. It can solve a set of kinetic equations describing the evolution of a system in time. It is available on mainframes or PCs, and is used mainly for kinetic modelling of large or small simulation problems. Modelling is carried out using a high level problem description language, which includes special features for: mass action kinetics, diffusion and advection, matrix and array operations, location of turning points and critical values, and a wide variety of output options. It is often used on non-kinetic problems. FACSIMILE contains a parameter fitting facility, for best fit of calculated results to observed data.

The program is used by a wide variety of organisations to solve a number of problems such as the modelling of:

- corrosion;
- radiation chemistry
- chemistry, photochemistry and transport of atmospheric pollutants;
- adsorption, resuspension and dispersal of maritime pollutants;
- transients in chemical and nuclear reactors, nuclear reactions in stellar interiors;
- flame propagation in internal combustion engines;
- fitting of chemical and biochemical reaction rate coefficients to kinetic data;
- signal propagation along a nerve axon;
- transients in, and phase/frequency response of, electronic circuits.

Consultancy on FACSIMILE applications is available.

FACSIMILE/HOWGOOD – enables one to assess the uncertainty in numerical values of results from almost any modelling program, arising from uncertainty in data values used by that program. It is an important tool for use in safety, design and quality assurance studies. It uses sophisticated sampling and analysis techniques.

Harwell Subroutine Library

The Harwell Subroutine Library is a collection of nearly 400 subroutines mostly written in FORTRAN, for assisting with numerical mathematical functions, linear algebra, numerical integration, approximation and data fitting, sorting, optimisation and solution of nonlinear equations. There is an extensive range of utility routines for IBM installations. Its particular strength lies in routines that exploit sparsity in many applications. Thus the subroutines are well suited for use in the solution of large-scale problems in science and engineering. Many of the routines have been modified so that they operate efficiently on vector computers, including Cray-2, XMP and Cray-1. In addition to commercial licences for individual subroutines a more restrictive but less expensive licence for the whole or part of the library has been distributed to over 700 organisations.

Oil Reservoir Simulation

Between 1976 and 1984 a Harwell team developed the general purpose three phase (oil-water-gas) three dimensional oil reservoir simulation software package – PORES. It is a fully implicit simulator which uses a finite difference formulation to solve sets of differential equations, with pressures and saturations the unknown variables, as a function of position and time. It enables the user to solve traditionally difficult problems such as high permeability contrasts, strong gravity segregation, small reservoir blocks, with high flow rates, wells completed in many layers and coning. PORES is available from Energy Resource Consultants Limited.

Mathematics
Information Systems
Advanced Computing and Knowledge Based Systems
Scheduling and Planning
Decision Support Systems
Software Engineering
Software Products

Information Systems

Easy access to information is the key to production commerce, administration, engineering and science. As the volume of useful information increases, many businesses and organisations are turning to the computer for help. However, computer information systems often deal only in figures and coded data, with the result that information becomes constrained to fit the computer program.

Harwell is one of the pioneers of text information storage and retrieval systems. Its STATUS package is marketed worldwide by Harwell Computer Power Limited and it is used by a variety of organisations for a wide range of applications. The package can also be used in conjunction with other software products to provide such facilities as graphical and statistical analysis, and with knowledge based systems to enhance the effectiveness of the search for information.

Information Management

The STATUS Information Storage and Retrieval software package provides users with facilities to store and retrieve data with great flexibility. It is capable of handling information ranging from totally unstructured (or free) text to structured numeric data. It is equally appropriate to the needs of the occasional user and the information specialist. STATUS can be used for simple data retrieval or as a component of a specialised information management; in the latter case it may easily be linked to other application-specific software. The package is largely machine independent and is installed on many different mainframe, mini and microcomputers.

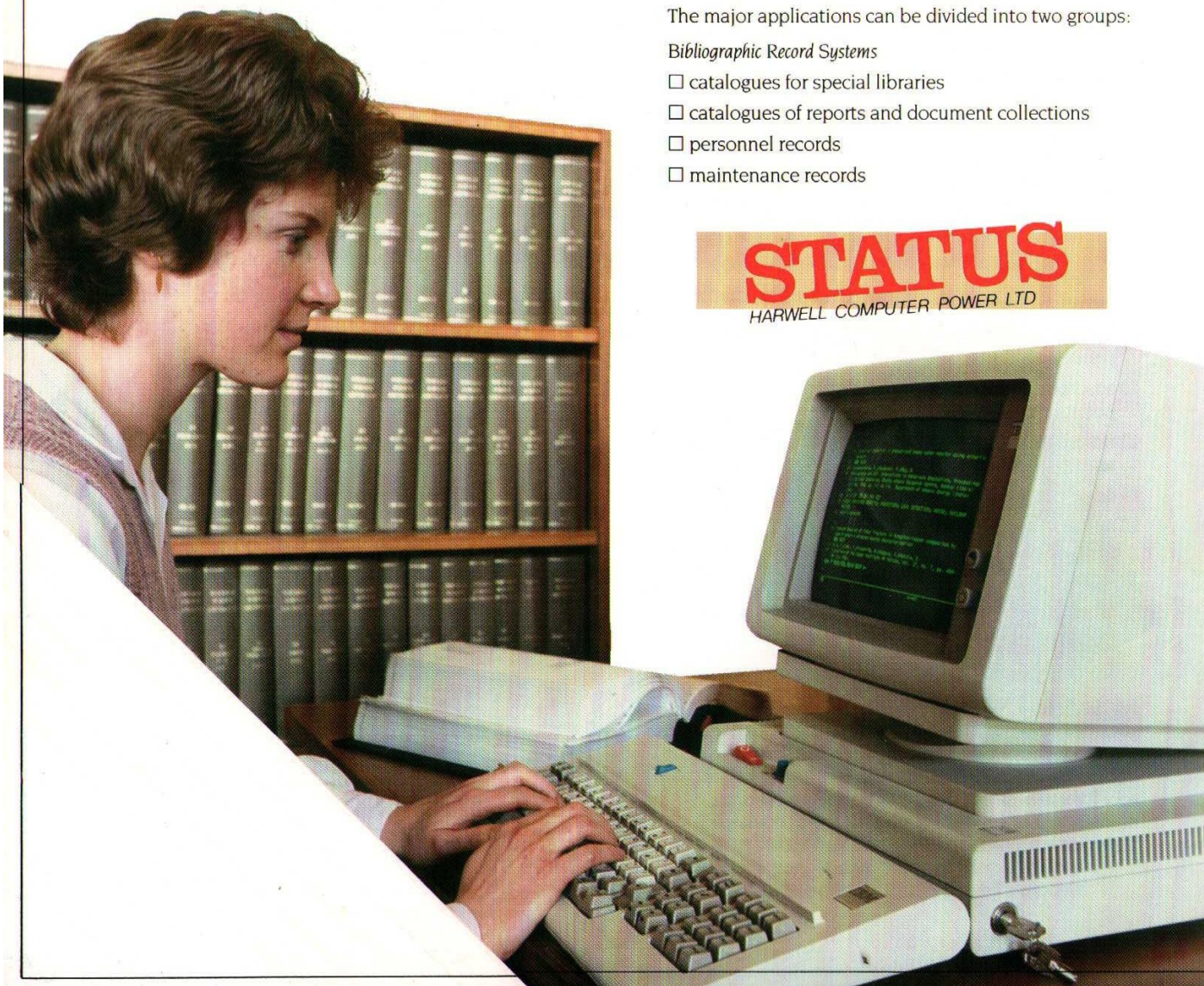
The flexibility of the STATUS free text system has resulted in its being used for a wide range of very different applications, even within one organisation. Advanced features allow the user interface to be tailored for specific applications without additional software.

The major applications can be divided into two groups:

Bibliographic Record Systems

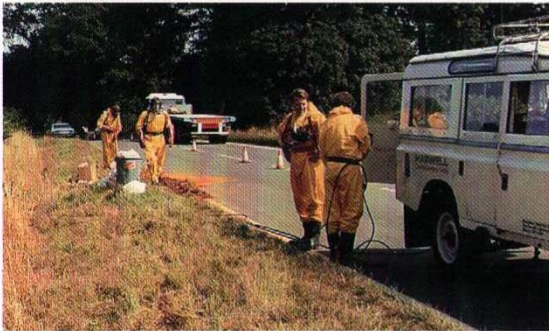
- catalogues for special libraries
- catalogues of reports and document collections
- personnel records
- maintenance records

STATUS
HARWELL COMPUTER POWER LTD



Full Text Systems

- legal statute, cases and related documentation
- documents in support of litigation
- technical reports, patents etc
- market intelligence
- accident or incident information systems
- office systems



Harwell's Chemical Emergency uses STATUS for the rapid retrieval of technical information from the hazards chemical database.

There are several public on-line services operating under STATUS and many organisations use this software on their mainframes and personal computers.

A major feature of STATUS is its ability to link readily with other parts of a total system without the need for further software development. Many applications involve an integrated Information Technology system with word processors, electronic mail, information storage and retrieval and report or bulletin production. Some recent applications consist of a knowledge base together with a STATUS text base. An expert system uses the knowledge base to provide consultancy to the user showing the appropriate information from the text base.

STATUS is marketed and supported worldwide by Harwell Computer Power and a network of appointed franchise holders. It achieved its 200th sale in 1986. Central support is now provided by Harwell Computer Power. This includes the provision of general specialised training courses for current and prospective users.

Computer Typesetting of Documents

Software has been developed for the preparation of documents which is particularly suitable for typesetting scientific literature. TSSD allows the user to control typeface, typesize and to format lines of text to a professional standard of typography. It performs automatic paging, multicolumn work, the floating of tables and boxing. A particularly useful feature is its ability to set mathematical expressions at any point in the text from a simple descriptive input language. Included is a powerful macro facility which allows the user to set up different house styles and to automatically generate indexes and contents lists.

TSSD can be readily used with many typesetters, including Pacesetter, APS-5, Linotron 202, Compugraphic 8400, IBM/3800 laser printer and Postscript devices. The interface between software and the user is independent of the characteristics of the typesetter. TSSD is in daily use on the Harwell computer and it has been installed by several customers. A version of TSSD for use on personal computers is being developed.

$$\sum_{i=\mu_0+1}^{\mu_0+m} C_n^i p^i q^{n-i} = \Phi(y_2) - \Phi(y_1) + \sum_{j=1}^{n-1} \frac{Q_j}{(\sqrt{npq})^j} + O\left(\frac{1}{n^{3/2}}\right)$$

holds as $n \rightarrow \infty$ for any fixed θ uniformly for $a \leq y_1 \leq y_2 \leq b$, where

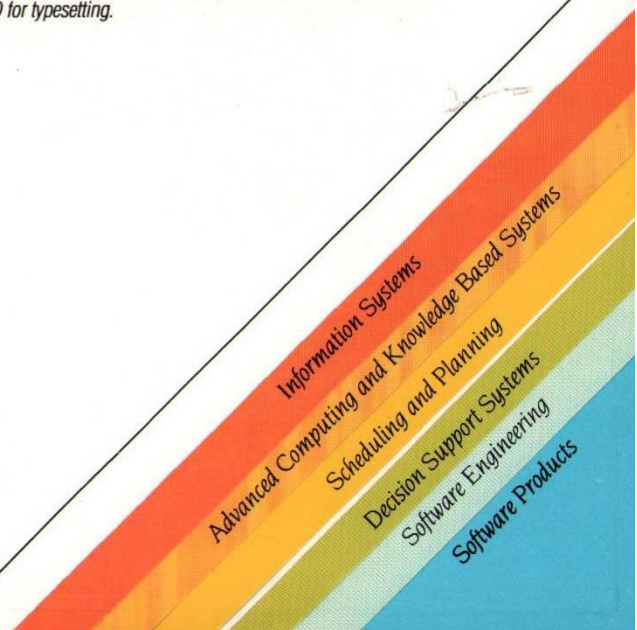
$$y_1 = \frac{\mu_0 + \theta - np}{\sqrt{npq}}, \quad y_2 = \frac{\mu_0 + m + \theta - np}{\sqrt{npq}}$$

$$\Phi(y) = \int_{-\infty}^y \phi(y) dy, \quad \phi(y) = \frac{e^{-y^2/2}}{\sqrt{2\pi}}$$

$$Q_j = -\frac{B_j(\theta)}{j!} H_{j-1}(y) \phi(y) \Big|_{y_1}^{y_2} + \int_{y_1}^{y_2} \phi(y) T_j(y) dy$$

$$+ \sum_{v=1}^{j-1} \frac{(-1)^v B_v(\theta)}{v!} \frac{d^{j-v-1}}{dy^{j-v-1}} \phi(y) T_{j-v}(y) \Big|_{y_1}^{y_2}$$

TSSD for typesetting.



Advanced Computing and Knowledge Based Systems

The application of techniques derived from research in the field of artificial intelligence is providing many new approaches to the development of computer based systems.

The use of high level, logic based programming languages is being investigated in several areas. These languages are powerful tools for implementing a number of applications ranging from system specification to equation solving and natural language processing.

An expert system environment SPICES has been implemented in PROLOG2 and provides flexible interfacing to other software systems, including graphics and information retrieval packages, such as STATUS. Knowledge based approaches offer a radical and effective method for the exploitation of Harwell's expertise in many scientific and technical disciplines.

Consultative expert systems have been developed on DEC VAX and PCs for a number of applications using the SPICES expert system environment and STATUS. The objective is to exploit technical expertise in problem solving, information transfer and training.

Intelligent knowledge based systems are being developed to provide advice on corrosion, adhesive bonding, non-destructive testing, electronic configuration and chemical plant design etc.



Expertise in seawater corrosion has been compiled as a knowledge based computer system.

Corrosion Applications

A number of Expert Systems for corrosion and corrosion control have been produced for the ACHILLES multi-company sponsored project.

The purpose of ACHILLES is to develop computer software tools to provide industry with the most appropriate information and advice from a database containing reports, data and other relevant information, to answer questions:

on Materials Selection, such as

What should any given component be made from?

How can it be protected?

How will it interact with other materials?

Will corrosion be the life-limiting factor?

and Failure Analysis, such as

What was the probable cause of corrosion?

What factors exacerbated the problem?

What remedial methods are available?

How can such problems be avoided?

It includes training to enhance the awareness of the practical applications by providing the knowledge in a structured highly interactive form which is directly responsive to the user.

The ACHILLES project is managed by the National Corrosion Co-ordination Centre in the UK, National Physical Laboratory, and is operated in conjunction with the Metals Technology Centre, Harwell Laboratory.

In addition to ACHILLES, the Harwell Laboratory has also developed under contract expert systems for corrosion of aircraft components and chemical plant corrosion.

Electronic Configuration

DENISE is an expert system and information base to assist in the selection of appropriate instrumentation for nucleonic counting applications based on the Harwell 6000 series of modular electronics.

Adhesive Bonding

ADEPT gives guidance on the selection and use of adhesives and on the design of effective adhesive joints. ADEPT incorporates access to manufacturer's data and stress analysis calculations on joint configurations. Comprehensive and expert design studies can be carried out in a single construction.

Chemical Plant Design

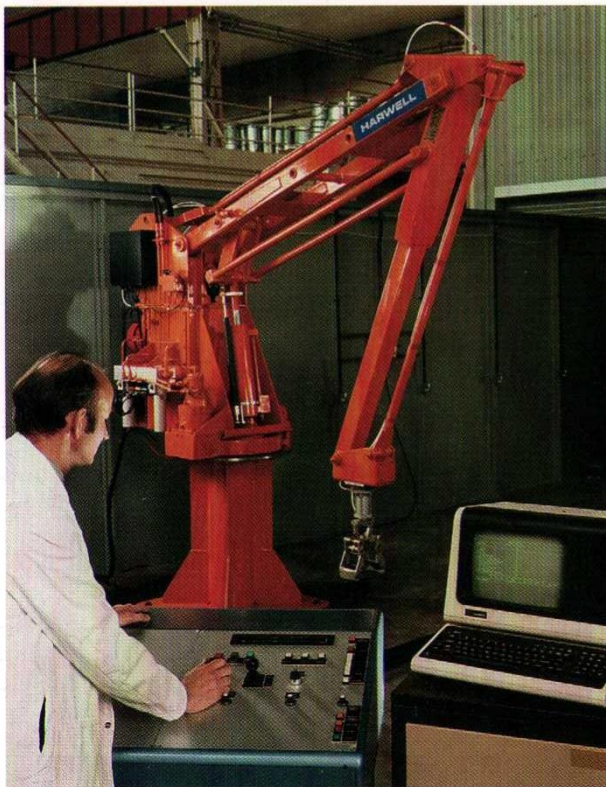
A prototype expert system has been developed to help engineers select solid-liquid separation plant by considering the process and feed properties. It will suggest suitable equipment and indicate problems that may arise:

New areas of research being explored by Harwell include:

Knowledge representation - techniques for knowledge processing based on adaptive networks and conceptual graphs.

Neurocomputing - Neural networks are based on theoretical models of how brain cells and their interconnections are able to perform exceedingly complex calculations. Particular areas of application are: knowledge representation, pattern recognition, image processing and optimisation techniques.

Robotics - The techniques developed for expert systems, knowledge representation and neurocomputers are being applied to studying advanced robotic systems, which are responsive to the environment in which they reside and can automatically adapt to new conditions, such as hostile environments, space, sub-sea and nuclear.



Computer controlled heavy duty handling machine used at Harwell for the deployment of decommissioning tools

Advanced Computing and Knowledge Based Systems
Scheduling and Planning
Decision Support Systems
Software Engineering
Software Products

Scheduling and Planning

Managers in both commerce and industry are concerned with evaluating the best use of their company's resources and with making realistic plans for the future. In the past, the size and complexity of commercial planning problems have frequently defeated the capabilities of classical operations research methods.

Harwell has gained a reputation for developing new and effective techniques for these traditionally difficult areas of planning, scheduling and production control. Harwell's policy of close collaboration with industry ensures the practicality and cost effectiveness of its work and has resulted in a record of successful implementations.

Major areas of expertise include:

Scheduling and Planning

Production scheduling, bulk carrier, oil tanker and cargo liners scheduling.

Control

Production control, contract management, project management.

Optimisation

Optimised layout for waste minimisation, resource allocation, optimised packing.



Major projects in this area include:

Workshop Scheduling and Planning

Designed for use by small batch manufacturing workshops and job shops, the WASP software analyses, plans and schedules variable workloads according to the availability of operators and machines. Better scheduling improves productivity, reduces costs and ensures target dates are met. WASP displays all shop floor loads and future schedules. It produces progress reports and planned completion dates for every job in hand. Jobs are scheduled in order of priority and very urgent work can be 'tagged' to displace other work already in progress (which will be reloaded automatically). The prime aim is to reduce queuing while maintaining high machine utilisations. As a result job throughput is markedly increased. Manning levels can be easily and quickly altered and predicted individual absences can be taken into account up to 52 weeks ahead.

WASP offers:

- Finite capacity schedules
- Full simulation of the workshop
- 'What if' schedules for planning and order acceptance
- Real-time interactive capability on VAX computers



Optimised Layout

Powerful optimising techniques have been developed for reducing the wastage when panels are to be cut from stock sheets of most raw materials, including printed circuit board laminates, timber, woodboard, plastics, glass and metal. These techniques are incorporated in the SHORTCUT software which:

- can handle a wide variety of cutting operations
- produces clear cutting patterns
- costs orders
- enables assessment of new sizes and sources of sheet
- is suitable for use with most cutting machinery
- makes appreciable savings in material costs and planning time

SHORTCUT has been developed in collaboration with the PCB and timber industries.

Similar techniques have also been applied to the three dimensional problem of packaging objects into cartons and storing the cartons on pallets, thus reducing warehouse space.



Strategic Planning and Scheduling of Shipping Fleets

FSP is a management system designed in collaboration with major UK and Scandinavian fleet operators. The primary functions of the system are:

- long term scheduling of the fleet
- budget prediction
- evaluation of business opportunities
- assessment of alternative programmes of fleet renewal and expansion

FSP is a package of programs that combines a comprehensive model of the shipping fleet with powerful software to construct economic fleet schedules and with an extensive range of reporting facilities. All normal transactions such as subletting time and chartering, and the taking of market opportunities are included. FSP includes its own database management system to give easy access to information on commitment, contract conditions, ship positions, past performance etc. Maintenance and retrieval of information is made very simple by the use of screen menus.

Similar techniques have been developed for scheduling the movement of goods by road.

Contract Manager

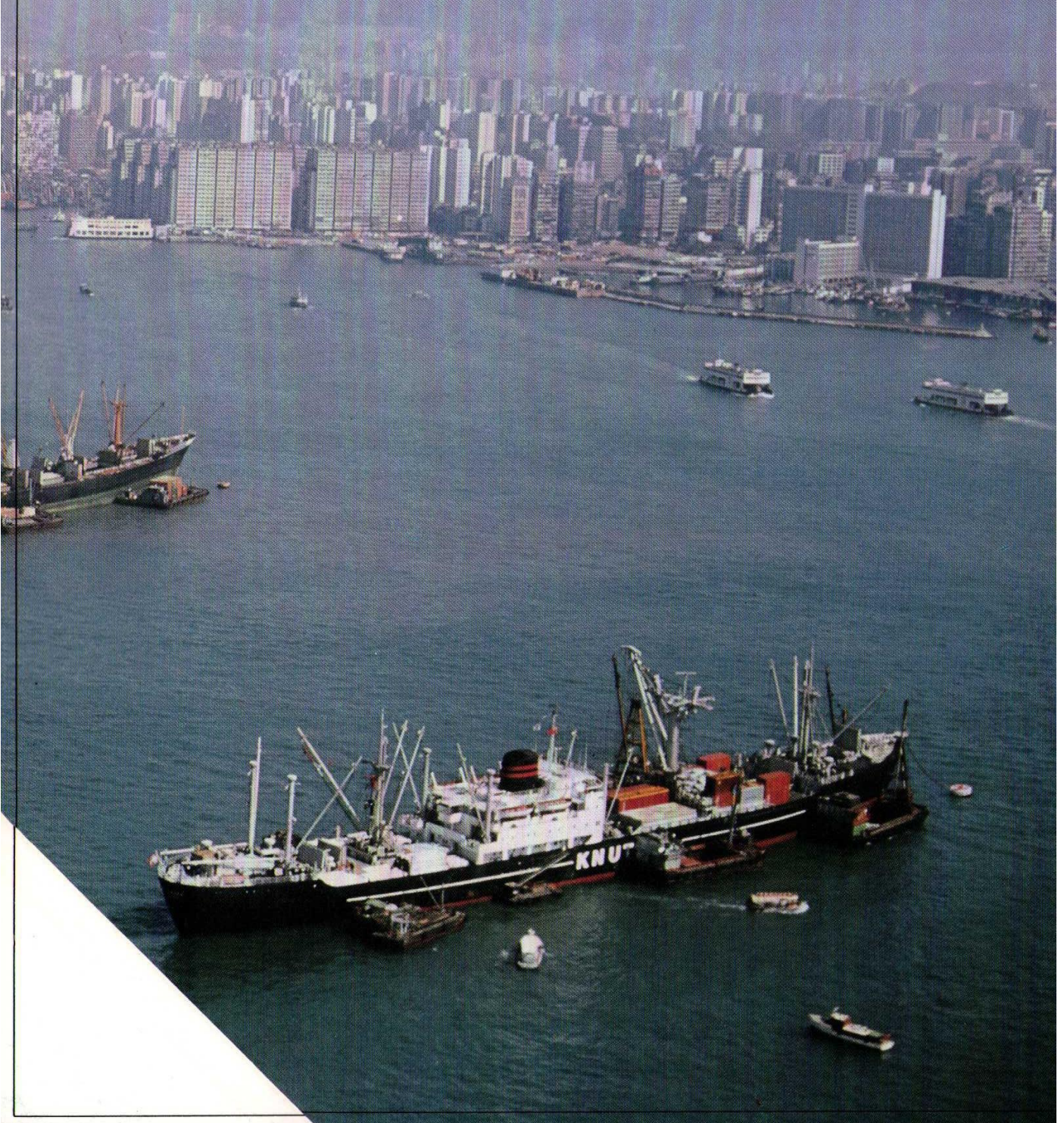
Software has been developed to monitor actions and obligations in progressing deliveries under highly complex uranium enrichment contracts. The inter-relationship between events such as the sampling of raw materials and the delivery of products are modelled using a simple language and articles from the enrichment contracts are collated into chronological diaries of events for the responsible managers.

Scheduling and Planning
 Decision Support Systems
 Software Engineering
 Software Products

Decision Support Systems

Decision support systems represent a new approach to the problem of interaction between the user and today's powerful and responsive computers. In such highly interactive systems the user occupies a central and controlling role.

Decision support systems are planning tools. They provide the manager with an integrated language of sub-models in order to gain a fuller understanding of the planning process. With these tools the planner may examine each aspect of his problem, test the sensitivity of subjective assumptions and evaluate the impact of a wide variety of scenarios.



Solid Waste Management

The Harwell Waste Management Model (HARBINGER) has been developed for the user to determine future policy on waste management. The program guides the user quickly and accurately through a sequence of operations. It is extremely flexible, allowing the waste manager to incorporate his/her own judgement and knowledge at any stage and to investigate what effect changing the data will have on the plan.

An integrated system of sub-models has been developed to address all the major elements of waste management:

- to forecast the types and quantities of wastes that will arise in the future
- to estimate transport costs (eg collection vehicles or bulk transport by road, rail, barge etc) including vehicles, labour and fuel, and to examine collection practice
- to cost new treatment and disposal technologies
- to cost alternative sites
- to calculate minimum cost disposal strategies
- to assess long term plans with their associated cost distribution, traffic implications and impact on the environment

Each sub-model is controlled through a simple language of commands which are supported by substantial in-built tutorial and menu facilities.

Although this decision support system has been specifically tailored to waste management, the techniques have general applicability to other capital investment and planning problems.

The model was first developed for the Hong Kong Government to determine future policy on waste management.

HARBINGER is available for installation on mainframes and a version can be used on IBM PC/AT computers.

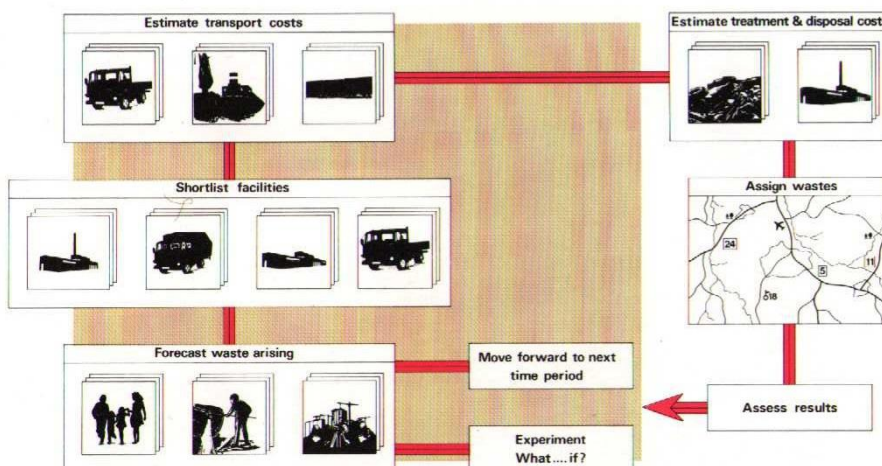


Uranium Enrichment Market Assessment

A system of programs has been developed as planning aids for a uranium consortium.

The capabilities of these programs include:

- exploration of demand for, and availability of, enriched uranium on a world wide scale
- scenario generation of demand and cash flow arising from the consortium's long-term contract.



Decision Support Systems
Software Engineering
Software Products

Software Engineering

The Computer Science and Systems Division develops and markets software packages for this purpose. The highly skilled work force undertakes consultancy, design and specialised systems development for industry. The Division has access to over 1200 scientists and engineers at Harwell who are specialists in a wide range of technologies and it is therefore well placed to develop systems to meet a broad spectrum of requirements.

These systems may embody the Division's software products or its proven expertise in:

- process control
- command and control
- data communications
- graphics
- man-machine interfaces
- highly reliable systems



Software engineering tools created by Harwell include:

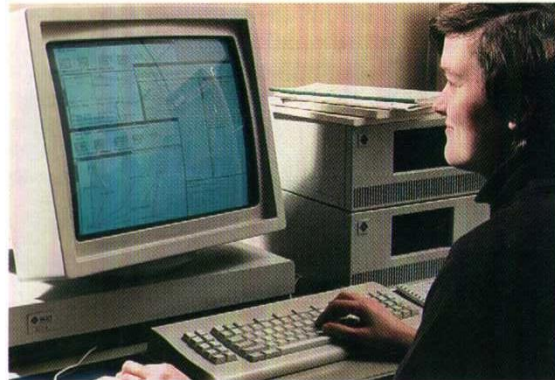
Program Development Facility

Interactive design using Jackson methods

PDF is an advanced software tool for the generation and maintenance of computer programs. JSP (Jackson Structured Programming) structures and program designs are built using PDF's interactive graphics. Structure diagrams and text are prepared and edited at the computer terminal prior to the automatic generation of the code. When requirements change, the structure diagrams are modified with PDF, thereby removing the need to maintain programs at source code level. The code may be generated in a number of high level languages including FORTRAN, PASCAL, PL/1, C, ADA, COBOL, JSP COBOL, CORAL 66 and RTL/2.

High quality documentation is a special feature of PDF. The user has full control over diagram pagination and can produce an extensive range of easy to use print-outs. As well as being a very useful tool for documenting JSP developments PDF can also be used for documentation of JSD produced software. Diagram output can be tailored to exploit capabilities of the more advanced printers.

PDF is available for installation and use on IBM PCs, VAX and IBM mainframes.

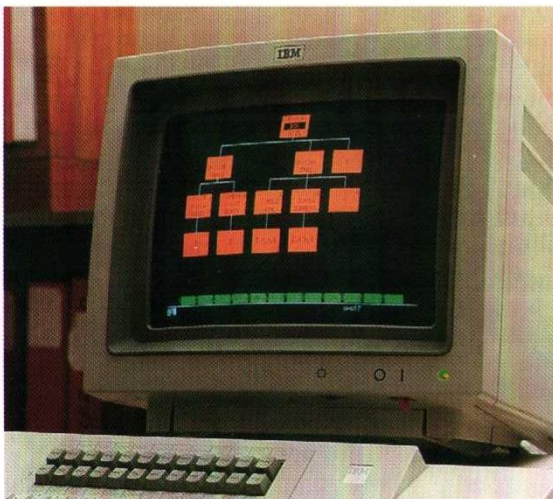


FOREST methods on a SUN workstation.

Formal Software Engineering Techniques

Significant improvements both in the increased quality of software and the reduced cost of its development can be obtained through the use of formal techniques throughout the software development cycle. These techniques are particularly valuable in the earliest stages of the development cycle, because errors in the specification tend to be discovered only after the full cost of designing and coding the system. Furthermore, the amount of re-work necessary to correct problems at this late stage can also be very high. This problem is especially acute in large real-time systems.

Harwell has collaborated with GEC Research, GEC Avionics and Imperial College (through an 'ALVEY' programme) in the FOREST (Formal Requirements Specification) development. Unlike many other projects on formal specifications, FOREST offers not only the logic framework for expressing specifications, but also a method for capturing the requirement, supporting software tools plus a training programme covering all three aspects. The tools are intended to run under UNIX on SUN workstations and are mostly written in C. Some support the method in assisting the capture, structuring and manipulation of information. They also check the consistency of that information. Others support the validation of the requirement specification, helping to ensure that it conforms with the real operational requirement. A third set are under development to support design and verification by transformations and theorem proving.



PDF for JSP methods.

Software Products

Research at Harwell into software engineering and developments has led to a number of applications software packages. Many of the programs originally written for the Laboratory's own use and for specific contracts are available commercially. The emphasis is on ease of use and flexibility to meet customer requirements. Licences to use these packages are available either directly from Harwell or through franchise holders.

Commercial Products Developed by Computer Science and Systems Division

FACSIMILE

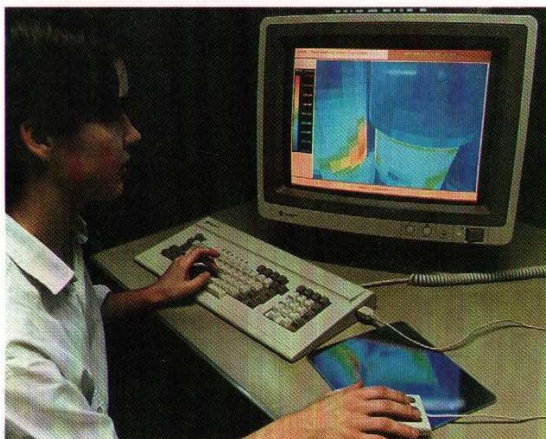
A suite of general purpose programs for simulating flow and chemistry which solve a set of differential equations. FACSIMILE/CHEKMAT (chemical kinetics with parameter matching) and FACSIMILE/CHEK (chemical kinetics without parameter matching) are both available for installation on a wide range of mainframe computers, including IBM, VAX, Prime, Hewlett Packard, and on IBM PC and compatibles.

FSP

Fleet scheduling program for planning the movement of fleets of cargo ships. It is written in FORTRAN for use on IBM mainframes operating in ISPF.

HARWELL FLOW3D

A general purpose code for the simulation of laminar and turbulent flow and heat transfer in and around complex geometries. Written in standard FORTRAN 77, FLOW3D can be installed on a wide variety of conventional mainframes and is well vectorised for use on supercomputers including Cray-1 and X-MP operating under COS and on the Cray-2 running under UNICOS.



FLOW3D used to predict the flow in the hot pool of the proposed design for the Commercial Demonstration Fast Reactor.

FTU

File transfer utility for transferring files between DECnet and IBM SNA networks. It is available from Scicon Ltd.

HARBINGER

An integrated set of sub-models for determining future waste management policies, including transportation, treatment and disposal. The software is available for use on mainframe computers and IBM PC and compatibles.

HARWELL SUBROUTINE LIBRARY

A collection of highly reputable subroutines for numerical methods of calculation. They are mostly written in standard FORTRAN and have been installed on a variety of computers. Vectorised versions of many of the routines are available for use on supercomputers such as Cray-1, Cray X-MP, Cray-2 and IBM 3090 VF.

HOWGOOD

A software tool, developed as part of the FACSIMILE suite of programs for analysing the uncertainty of results due to uncertainties in the input data to a modelling program. It is available for use on IBM PC and compatibles, and is marketed by ARC Scientific Ltd.

PDF

Program development facility for the generation and maintenance of software written to Jackson methods of programming. Versions of PDF and the code generators are available for installation on VAX/VMS, IBM/MVS, IBM PC and compatible computers. The software is available from Michael Jackson Systems Ltd. and Systems Designers plc.

PORES

A general purpose three-phase (oil, water, gas) three dimensional simulator of oil/gas reservoirs. PORES is marketed by Energy Resource Consultants on behalf of British Gas, Britoil and UK Department of Energy.

SHORTCUT

For minimising waste produced when cutting panels of printed circuit boards, wood, metal, plastics, glass etc. from sheet material. SHORTCUT is for use on IBM PC and compatibles. It is available from Harwell and a number of franchise agents in the UK, USA and other countries.

SNAPI

Systems Network Architecture Performance Indicator for the efficient use of computer terminals. SNAPI is marketed by Tessella Support Services Ltd.

SPICES

A collection of logic programming tools for the construction of knowledge based systems. The tools are mainly written in PROLOG but provide access to code written in other programming languages and to free text and relational database systems. SPICES is available for use on VAX computers and IBM PC compatibles.

STATUS

Free text information storage and retrieval system for use on a wide variety of mainframe computers and IBM PC and compatibles. STATUS is available from Harwell Computer Power Ltd. and many franchise agents around the world.

SUPERGATE

IBM-DEC link via Systems Network Architecture.

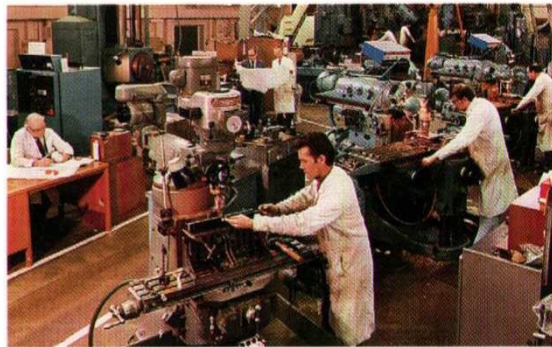
SUPERGATE provides a high speed gateway between DECnet and IBM (SNA) networks enabling non-IBM devices on DECnet to connect to IBM host services. SUPERGATE runs in a PDP11 processor which is simultaneously a DECnet node and a Physical Unit Type 4 Communications Controller channel-attached to an IBM mainframe operating SNA protocols. SUPERGATE was developed jointly with Scicon Limited who market the product.

Supergate emulates a sub-area of an SNA network consisting of terminal clusters connected through an IBM 370X communications controller.

A version of SUPERGATE, XN4000, has been developed at the Science and Engineering Council Establishment at Daresbury for General Electric 4000 series computers.

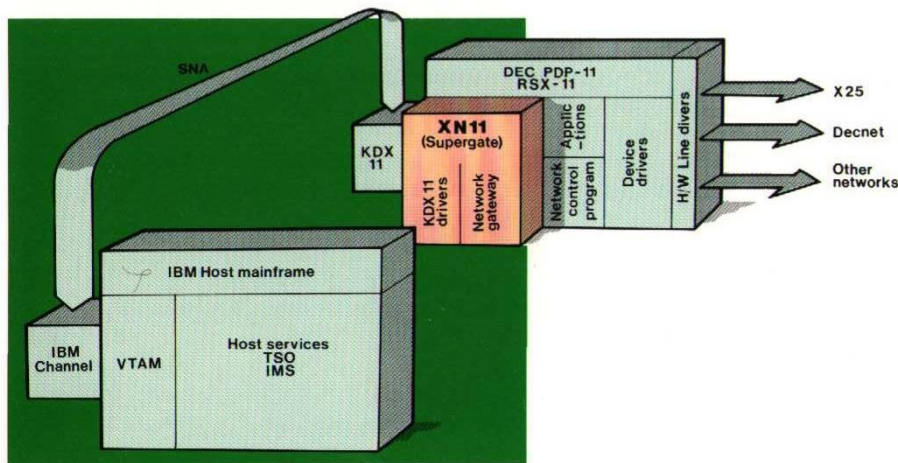
TSSD

Typesetting of scientific documents including the reproduction of complex mathematical formulae for use on VAX and IBM mainframe and IBM PC and compatibles. TSSD will produce output for a variety of equipment, including Postscript devices, IBM laser printers, Linotron 202 typesetters and others.



WASP

Workshop analysis, scheduling and planning package for small batch manufacturing and 'made to order' work. WASP has been installed on a variety of mainframes, including IBM, DEC, ICL and Prime. PC-WASP is written for use on IBM PC and compatibles. The software is available from Harwell and a number of agents in the UK, USA and other countries.



Computing Technology for Industry

Computer Science and Systems Division's Customers Include

AKZO (Holland)
Alcan Ecko Ltd
American Express Co
Amoco Products Co (USA)
Arco Metals Corp (USA)
Arnold Laver Ltd
ASEA (Sweden)
Associated Nuclear Services
Atomic Energy of Canada Ltd
Attorney General's Department (Australia)
AWRE

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Battelle (USA)
Bahrain Petroleum Co
Binnie and Partners
BNF Metals Technology Centre
Boart Hardmetals (Eire)
BOC Ltd
Bohannon-Huston Inc
Boeing Computer Services (USA)
BP Exploration Ltd
British Aerospace plc
British Gas plc
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British Technology Group
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Building Services Research and Information Association
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Burma Oil Exploration Ltd
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CAD Software Inc (USA)
Central Electricity Generating Board
Century Research Centre (Japan)
CH2M Hill (USA)
CI Industries Ltd
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Geo Strachan & Son Ltd
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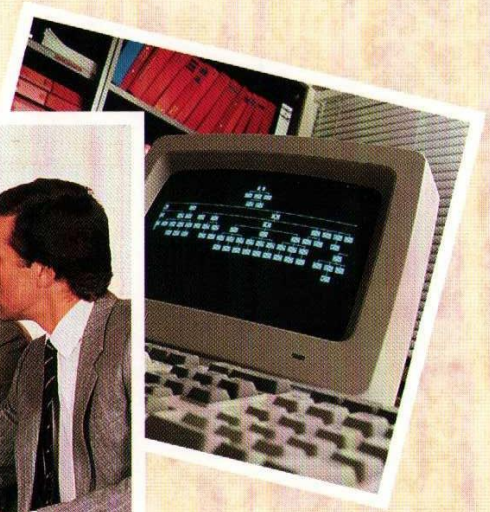
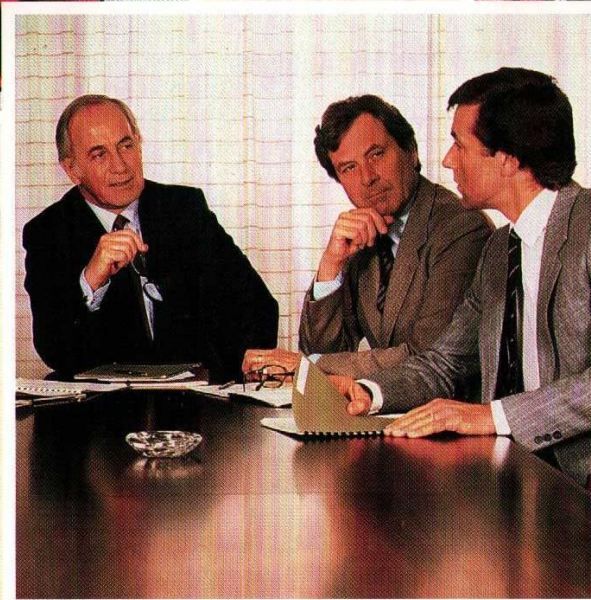
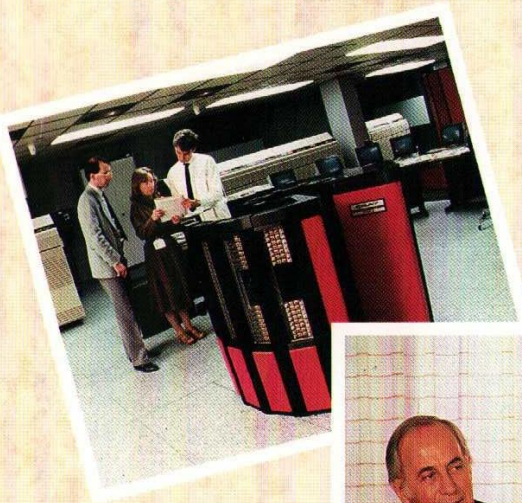
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 University of Southampton
 University of Tokyo
 University of Trondheim
 Urenco Ltd
 US Air Force

Vickers Ltd

WS Atkins Group
 Wellcome Foundation Ltd
 West African Bulk Services
 Westborough Computer Services
 William Browns Sawmills Ltd
 Woolworth (Australia)

Further Information



Tony Stone Worldwide

For further information on any of the services discussed in this brochure please contact:

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