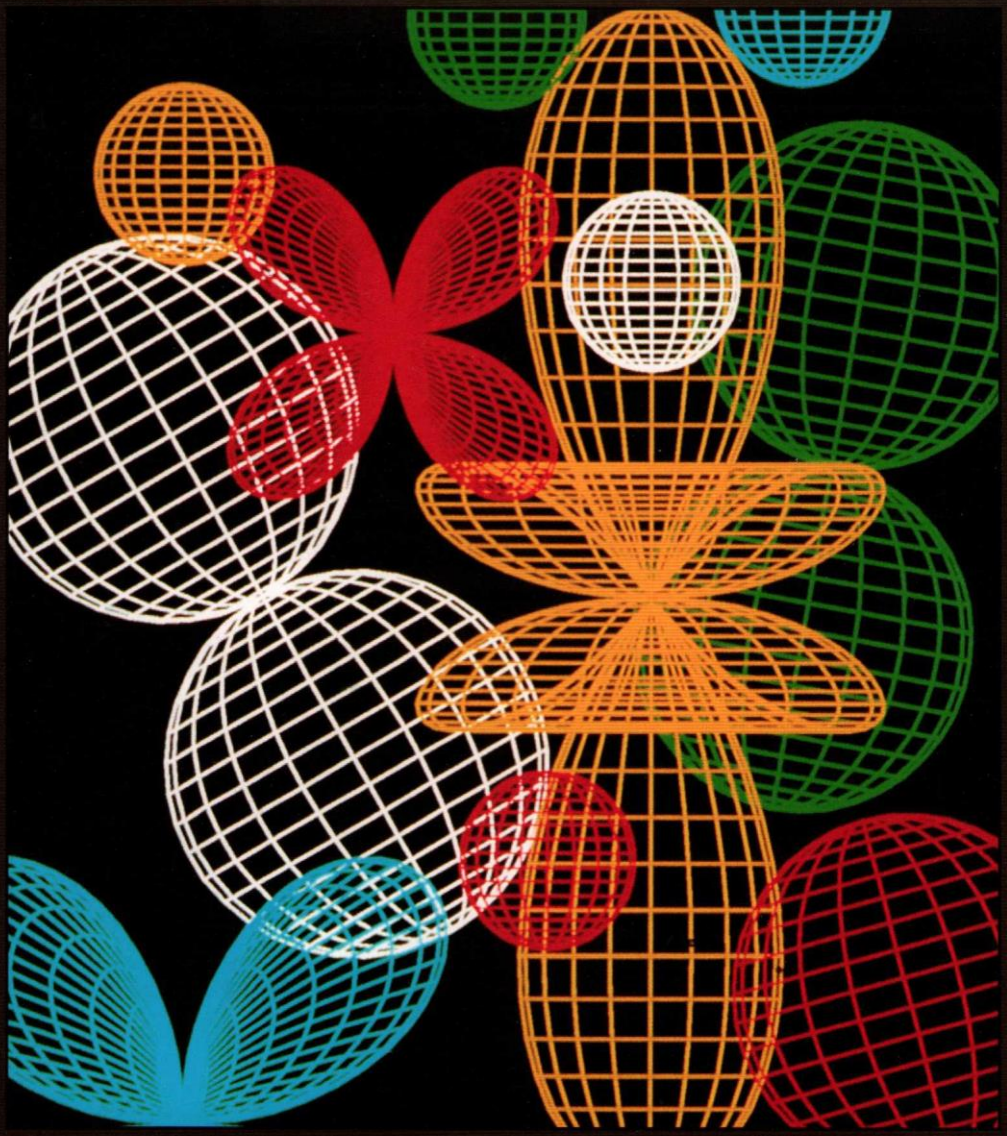
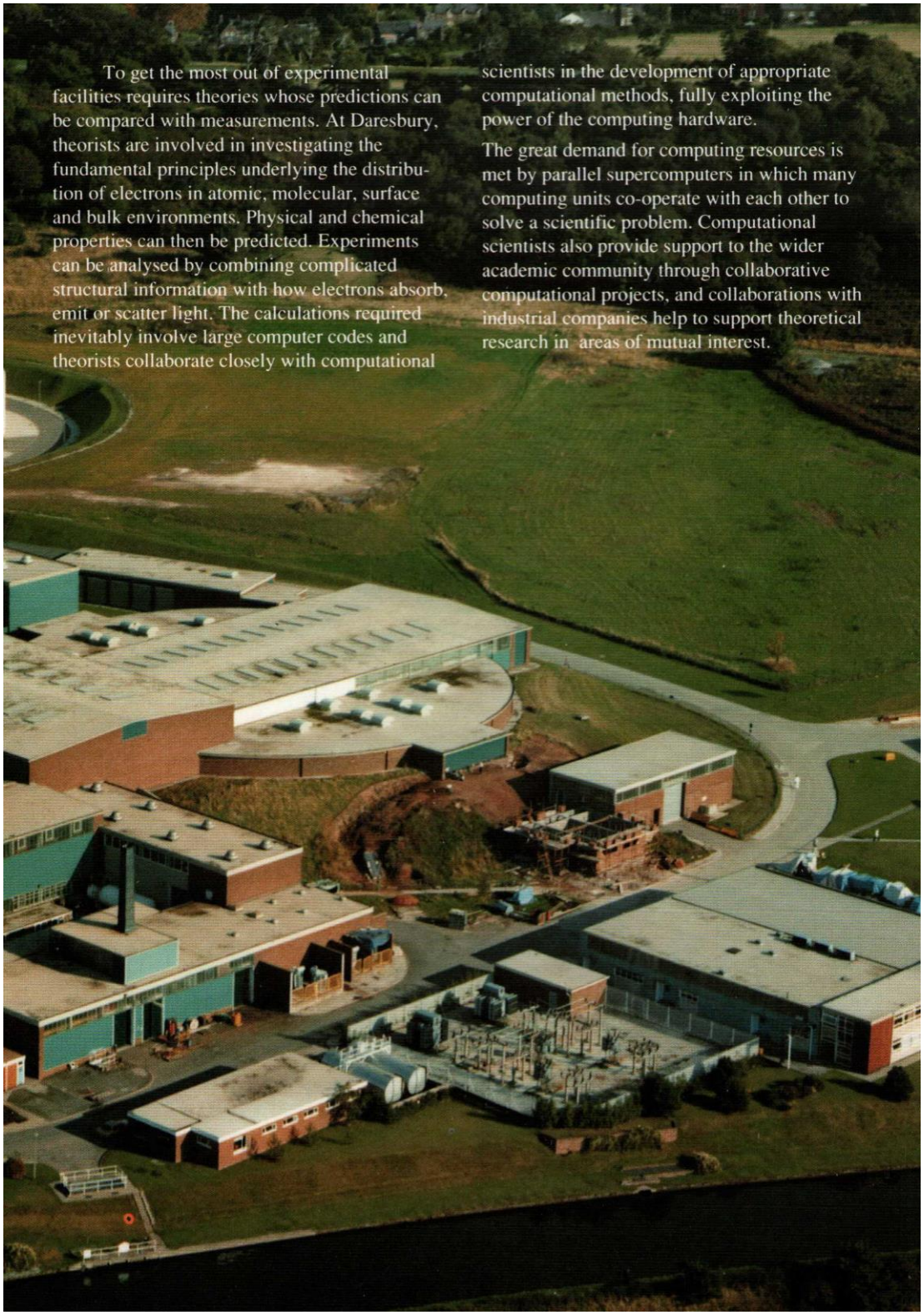
THEORY AND COMPUTATIONAL SCIENCE



DARESBURY LABORATORY

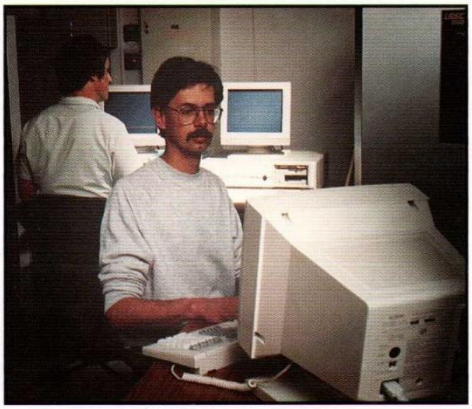
To get the most out of experimental facilities requires theories whose predictions can be compared with measurements. At Daresbury, theorists are involved in investigating the fundamental principles underlying the distribution of electrons in atomic, molecular, surface and bulk environments. Physical and chemical properties can then be predicted. Experiments can be analysed by combining complicated structural information with how electrons absorb, emit or scatter light. The calculations required inevitably involve large computer codes and theorists collaborate closely with computational scientists in the development of appropriate computational methods, fully exploiting the power of the computing hardware.

The great demand for computing resources is met by parallel supercomputers in which many computing units co-operate with each other to solve a scientific problem. Computational scientists also provide support to the wider academic community through collaborative computational projects, and collaborations with industrial companies help to support theoretical research in areas of mutual interest.



Theory and Experiment

Scientific research at Daresbury is supported by the expertise of theory and computational scientists. Theories exploiting the fundamental principles of physics are translated into sophisticated computer programs to run on powerful computers, permitting the understanding of experimental results



or the prediction of new phenomena. Assistance of this kind is indispensable in the analysis of data generated by the Synchrotron Radiation Source (SRS) which is primarily concerned with the interaction of electromagnetic radiation (light) with matter.

The discovery of new effects, and the development of new theories to explain them, inevitably leads to a demand for more computing power and new computer architectures are continually emerging to meet this need. In addition, new computational methods, such as computer graphics, are required to help interpret the data. Scientists at Daresbury are making valuable contributions in these areas.

Computational Science

Computational science is largely orchestrated through a series of Collaborative Computational Projects (CCPs), each of which focuses on a specific area of research .The CCPs assist the universities in developing, maintaining and distributing computer programs and promoting the best computational methods. The projects are funded by the Science and Engineering Research Council and

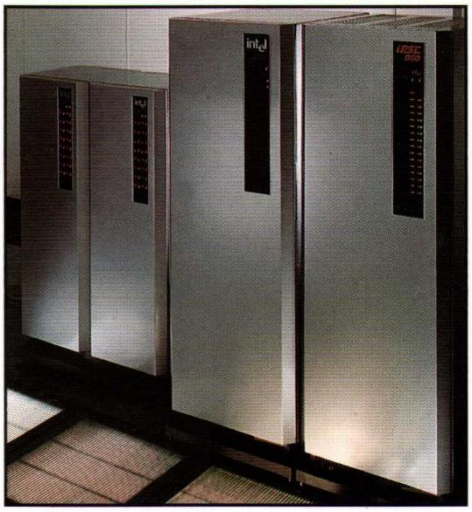
CCP1	Correlated wavefunctions
CCP2	Continuum states of atoms and molecules
CCP3	Computational studies of surfaces
CCP4	Protein crystallography
CCP5	Computer simulaton of condensed phases
CCP6	Heavy particle dynamics
CCP7	Analysis of astronomical data
CCP9	Electronic structure of solids
CCP10	Plasma physics
CCP11	Biosequence and structure analysis
CCP12	Computational fluid dynamics

most of them are scientifically supported by Daresbury Laboratory.

Daresbury also collaborates with industry. A joint project with ICI supports theoretical and computational methods in studies of polymers, catalysis and pharmaceuticals.

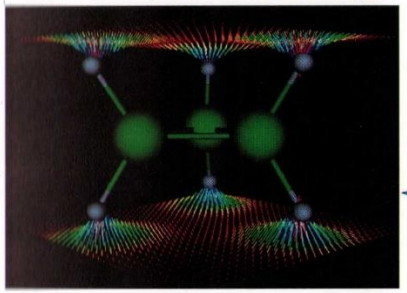
Advanced Research Computing

The Daresbury Advanced Research Computing Group is concerned with the most modern aspects of scientific computing; work is directed specifically towards the newest and most advanced computers available. These include 'parallel computers', such as the Intel iPSC/860, which currently has 32 processing nodes, each one capable of 40 million multiplications in one second. Such computers herald a new age in computing and promise to keep the Laboratory at the forefront of computational science.



Scientific Research

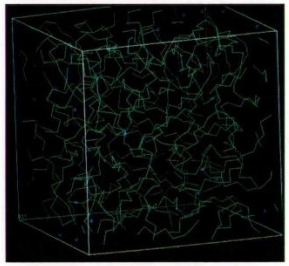
Quantum chemistry (the field of CCP1) describes the chemical bonding in molecules through techniques such as molecular orbital and valence bond theory. Large and powerful computers are required



Quantum Chemistry

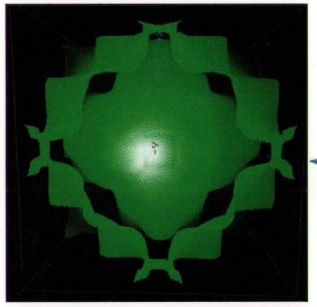
to perform the highly complex calculations necessary to give accurate results comparable with experiments. The results are particularly important to spectroscopic studies of molecules.

Molecular simulation is supported by CCP5 and investigates the bulk behaviour of molecules using techniques such as molecular dynamics and Monte Carlo simulation, which are computationally demanding. A knowledge of the forces between molecules makes it possible to predict the structural and dynamical properties of the bulk materials they make up. This has important applications in studies of liquids, solids, plastics, biopolymers, drug manufacture and catalysis.

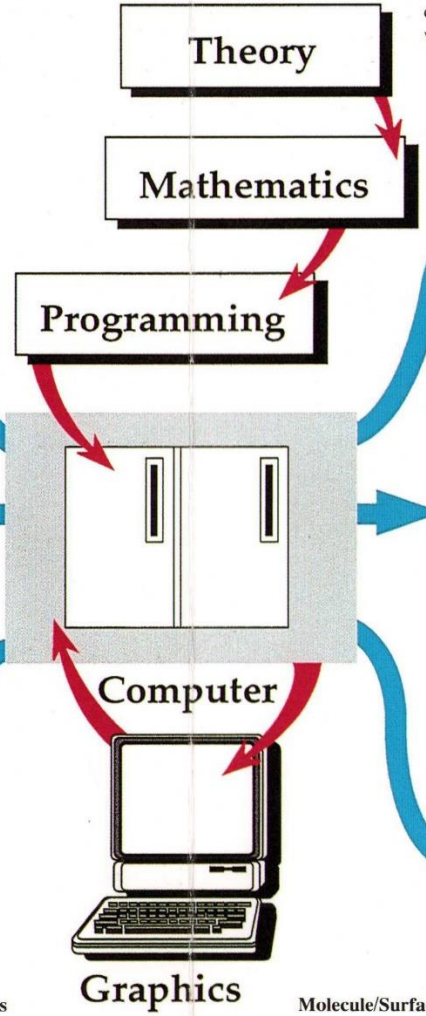


Molecular Simulation

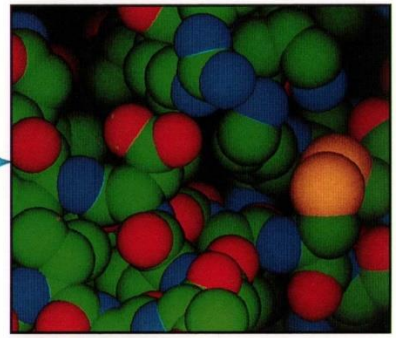
Solid state physics is founded on the electronic structure (band theory) of important materials such as semiconductors, high temperature superconductors and catalytic surfaces. The most common band theory techniques applied are density functional theory and Hartree-Fock theory. There is also a strong interest in the properties of crystalline materials for which energy minimisation methods are most popular. These studies are pursued by CCP3, CCP5 and CCP9.



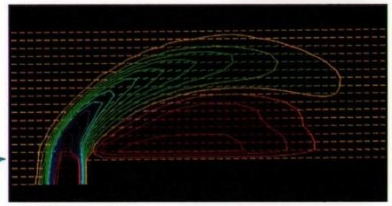
Solid State Physics



Protein Structure is determined using the x-ray diffraction resources provided by the SRS. The definitive molecular structure of protein crystals is obtained from diffraction patterns which can only be analysed by intensive computations and this work is undertaklen by CCP4. The relationship between the protein amino acid sequence and the structure adopted by the protein in nature (the tertiary structure) is supported by CCP11.

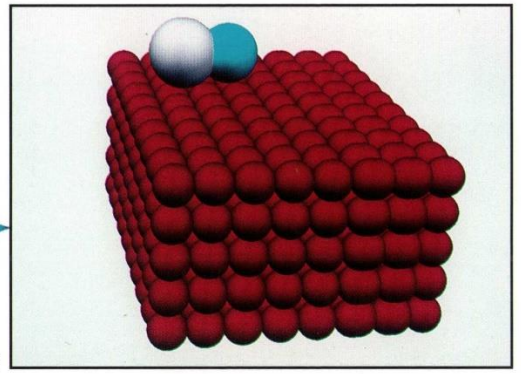


Protein Structure



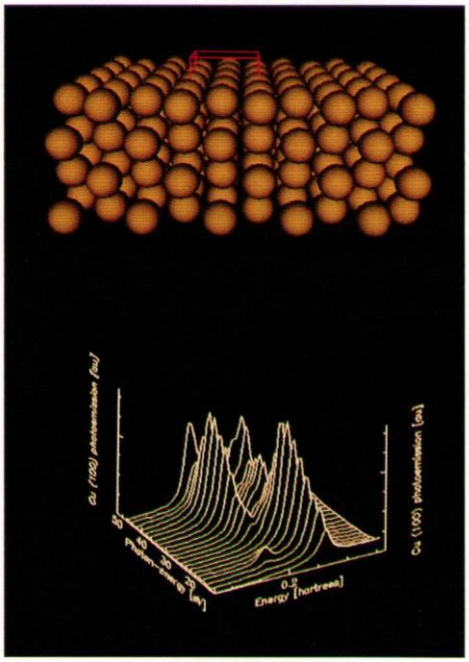
Fluid Dynamics

Computational fluid dynamics models how fluids flow past obstacles and is an important engineering study. The flow is described by the Navier-Stokes equation which can only be solved numerically. Vast computing resources are required and CCP12 has been created to exploit parallel processing and computer graphics in this and related fields in engineering.



Molecule/Surface Scattering

Atomic and molecular scattering deals with collisions between molecules and atoms which occur in many natural processes. During such collisions, an atom approaching a molecule or another atom at high speed may knock out or capture electrons, thereby effecting a chemical reaction. Theoretical results from this work are used in models of plasmas and in astrophysics. CCP2, CCP6 and CCP7 support this work.



Scientific Databases

SEQNET is a service for molecular biologists. It allows on-line access to all the major protein and nucleic acid sequence databases and receives nightly updates for EMBL and GenBank databases. The service also provides biological macromolecule structure databases such as Brookhaven. A large array of other user databases inlcudes information on cloning vectors, genetic maps, gene designations and structural features. SEQNET also contains a host of programs and software packages for data retrieval and analysis, covering such diverse areas as sequence similarity analysis, DNA sequencing and phylogeny.

The Chemical Databank Service (CDS) provides online access to a dozen chemical databases including crystal structure, metals data, electrolyte solutions, NMR data, organic reactions and synthesis and a fine chemicals directory. Facilities are available for connectivity searching some of the databases, the graphical display of structures and the analysis of numerical data.

The SEQNET and CDS national services are provided by the Scientific Database group.

Computer Hardware

Computational scientists have access to a wide variety of powerful computers which are linked via the Laboratory-wide ETHERNET and to the Joint Academic Network (JANET);

CONVEX C220 minisupercomputer
FPS M64/60 attached processor
MEIKO Computing Surface
INTEL iPSC/2 parallel computer
INTEL iPSC/860 parallel computer
ARDENT TITAN 2 graphics workstation
APOLLO DN10020 graphics workstation
SILICON GRAPHICS 4D/220GT graphics workstation

DARESBURY RESEARCH SERVICES

Daresbury Research Services (DRS) aims to improve the interface between science and industry by offering access, on a commercial basis, to the Laboratory's unique scientific facilities. DRS offers a speedy and highly confidential service to industrialists who seek the availability of both world class equipment and scientific expertise.

The Laboratory provides access to the SEQNET (Molecular Biology Database Service) for commercial users. As well as access to databases and packages, support is provided with computing problems and, where possible, biological queries.

In addition, access is also available to the ELYS Electrolyte Solutions database (Chemical Databank Service) which contains thermodynamic and transport properties

Enquiries

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Where is Daresbury Laboratory?

Conveniently situated close to the motorway network in North Cheshire (Junction 11 on theM56), the Laboratory is also accessible via Inter-City rail links (Warrington or Runcorn) or from nearby airports at Manchester or Liverpool.
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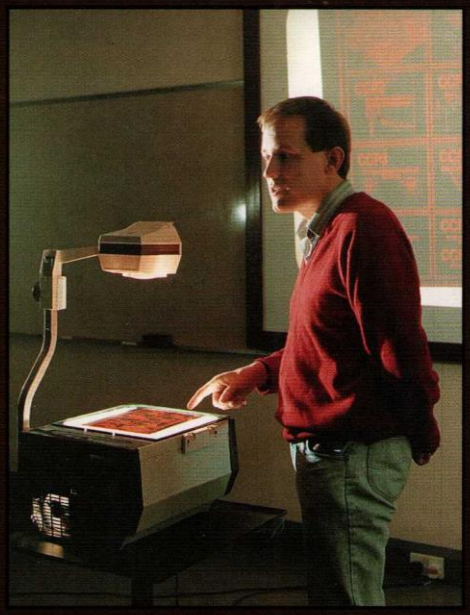
(Telex Number 669581) provide a Bureau Service and will transmit telexes to the Laboratory on request.



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