in progressing algorithmic research. For we often find that developing more efficient ways to carry out some computation rests on understanding the physics of the phenomenon under study. In my own field of research, one of the most demanding computations consists in the calculation of quark propagators in the background of a non-uniform gauge field, which must be carried out many times to simulate quantum fluctuations. In mathematical terms, the calculation consists in solving a very large system of linear equations (with a number of variables that can reach into the millions), with a matrix of coefficients which is very sparse, but non-uniform and with poor-quality condition numbers. Ideally, one would like to apply multigrid methods or other acceleration techniques. What one sees is that the ability to implement such methods is closely coupled to understanding the physical properties of the lowest eigenstates of the quark field, so algorithmic progress and progress in unravelling the physics go hand in hand. Issues of physics and computing are not separate, but should be seen as complementary.

#### **Putting into Practice**

There is an emerging consensus that computational physics should be taught at the undergraduate level. This is a difficult challenge. An undergraduate course on advanced computing in physics based on the matrix approach was given for the first time last year at Boston University as part of a coordinated set of new undergraduate courses on parallel computing supported by the US National Science Foundation. Some of the projects used in the course are summarised in the insert.

My experience in teaching the course was that I assumed too much about the students' background preparation. This is a real difficulty because teaching computational physics must proceed concurrently with the rest of the curriculum. One way to help solve the problem is to use the tools whose utilization we wish to teach as the basis for making many mathematical concepts accessible. For instance, the notion of a Laplacian operator can be introduced using image manipulation procedures. The idea is to start with pixels that form an image and blur the image by replacing their numerical values with the averages of their neighbours.

A more serious — and I believe general problem is to make room for new courses in an already overcrowded curriculum. Exposing students in general courses to computational projects is not a solution because there is much more to the methodology of computational physics than seeing the results of its applications. However, by cleverly integrating the power provided by modern computational tools in the overall curriculum we may be able to help students acquire more easily all of the many notions that are indispensable for a physicist.

This text is taken from an invited talk given by Claudio Rebbi at the 6th Joint EPS-APS International Conference on Physics Computing (Lugano; 22-26 August 1994) and published in the proceedings.

### PC'96: 7th JOINT EPS-APS INTERNATIONAL CONFERENCE ON PHYSICS COMPUTING

Pittsburg, PA, USA	June 1996
Contact: D. Barnes, LANL	

## **1997 IUPAP Computational Physics Conference**

The International Union of Pure and Applied Physics (IUPAP), in reappraising its role, decided at its General Assembly last year in Japan to explore the possibility of forming a Special Commission for Computational Physics. A working group was set up which will shortly present a proposal to IUPAP's Executive Committee for the new Commission (the Executive has the authority to establish the Commission).

It is proposed that the Commission should adopt a broad perspective by promoting "the exchange of information and views among members of the international community of physicists in the area of of computational studies of problems related to physics including:

- numerical and symbolic models and algorithms for simulating physical systems;
- computational control and data processing in experiments;
- computing environments;
- the physical basis of computing machinery."

The new Commission also sees itself as the body that sanctions international conferences in the field of computational physics. The working group has therefore agreed with representatives of the various regional physical socie-

ties that a IUPAP-sponsored conference should be held every three years, with the joint EPS-APS conference alternating during the intervening years. Consequently, the next joint EPS-APS conference (Physics Computing '95) will be held next in Pittsburg, followed by PC '96 in Cracow with the IUPAP event in 1997 in Beijing.

## SUPERCOMPUTING CENTRES

# A Variety of Approaches

Supercomputing facilities in the various east and central Europe are evolving at different rates in the various countries, with Poland adopting the most adventuresome attitude.

#### POLAND

Poland's main supercomputing centre is the Academic Computing Centre based in Cracow's Institute of Computer Science. It was established some 20 years ago and now serves 11 institutes in Cracow, but following a recent policy change it will see its user community grow to include other institutes. Most investments have been funded by the State Committee for Scientific Research (KBN) which runs the country's research grants scheme (see EN, April 1994). The most recent investment is an agreement signed a few months ago to purchase one of Convex's latest generation of massively parallel supercomputers (a 16-processor machine in the Exemplar series that offers scalable parallel processing with from 1 to 128 central processing units). The Centre already has three Convex machines, the first of which - and the first Convex in central and eastern Europe - was acquired about four years ago. Some six other Convex computers are distributed around the country (in Torun, Warsaw University, the Oil and Gas Institute in Cracow, the Institute of Nuclear Physics) and two are in industry.

Warsaw's Centre for Scientific Supercomputing based at the Institute of Applied Mathematics, Computer Science and Mechanics of the Polish Academy of Sciences is equipped with a so-called "baby" Cray (an 8-processor machine in the Cray Y-MP EL series with up to 32 CPUs). Warsaw University also has a computing centre based on an IBM 3090 which was delivered in 1990 to form an European Academic Research Network (EARN) node — the first in east and central Europe — as part of IBM's Central European Academic Initiative. There is a computer centre attached to the Polish Academy of Sciences Institute of Biology in Poznan which acquired a 4-processor Cray Y-MP EL this year. The *KBN* recently signed an agreement with Cray for 6.5 M\$US to be spent over 2 years to upgrade supercomputing resources.

## **CZECH REPUBLIC**

The Institute of Physics of the Czech Republic's Academy of Sciences acquired a Cray Y-MP EL in 1992. Owing to financial constraints, it has proved difficult to develop a large user base (users are concentrated in physics, with most coming from universities). The Institute recently formed a consortium to seek support from the Czech government's Foundation for the Development of Science to build up a National Centre for Supercomputing that would be in a position enlarge its client base and support by working for industrial companies. These could include US firms that have been contracted by the government to upgrade Soviet-designed nuclear reactors. The immediate need is to increase the number of workstations and improve software resources. However, a project along these lines was not approved this

A deskside Y-MP EL Cray supercomputer.





David Andersen from California who chairs IUPAP's computational physics working groups.

year so pending a re-application, the emphasis is now on establishing firmer links with three computing centres in the universities (among them being the centre at the Czech Technical University which has the IBM 3090 supplied in 1991 under IBM's Academic Initiative). The difficulty to establish a feepaying clientele for a supercomputing centre is demonstrated by the fact that the country's weather services prefer to carry out much of their computing abroad at something like five-times the cost.

## **NEUTRON SCATTERING**

## **Representatives Opt for a Federation**

The various national organizations representing users of neutron sources have set up a representative body of delegates called the European Neutron Scattering Representation committee. It met for the first time on 5 September in Grenoble and elected D. Richter from the KFA Jülich as the interim chairman. The committee's main task is to decide upon and implement the best form for future representation for Europe's neutron scattering community. Various options were discussed and following a vote it was agreed to aim for a federative structure whereby national organizations would nominate delegates. However, the advantages of a representative society to which Europe's neutron scatterers could belong were clearly recognized, so it was also decided to aim in the long term at forming a European society.

Norbert Kroó, the EPS President, argued vigorously for an EPS Interdivisional Group as this would provide a solid legal framework, strong links to other organizations, full representation of members, close involvement in established conferences and publications, and low secretariat costs. The major difficulty seems to be that EPS largely represents physicists while neutron scattering involves scientists from other fields (some 35% of Europe's 1400 neutron scatterers are che-

### HUNGARY

Hungary's work in advanced computing was traditionally carried out at the Computation and Automation Institute of the Hungarian Academy of Sciences in Budapest. The main change occurred when Budapest's University of Economic Sciences acquired an IBM 3090 under IBM's Academic Initiative for its Budapest University Computing Centre on the condition that an academic network was built up (this is being done under the national Information Infrastructure Development Programme). There has has been a tendency to concentrate resources at the workstation level as it is acknowledged that this level cannot be ignored. A true supercomputing level of the Cray or Convex class is missing and there appears to be no definite plans to change this. Computational physicists therefore tend to work abroad, with some questioning whether this is particularly cost-effective.

P.G. Boswell

## Main Issues Identified

mists and 10% are biologists). However, R. Scherm, the ILL's Associate Director who becomes the Director on 1 November (replacing J. Charvolin who was Director during the refurbishment of the ILL's reactor), feels that physicists often play a key role since they must increasingly make neutron easily available to users with a variety of backgrounds and interests. So it is not unreasonable for physicists to take the lead. Second, the Interdivisional Group concept has shown in the case of computing and control systems that it can cater very successfully for the multidisciplinary aspects of science while providing the advantages of full representation. A task force composed of F. Barrochi

(Florence University), C. Carlile (Rutherford-Appleton Laboratory), A. Furrer (PSI, Villigen), D. Richter (KFA, Jülich), and T. Tasset (ILL, Grenoble) was formed to draft statutes for a new organization. The committee itself will next meet on 11-12 December in Madrid.

#### NATIONAL ORGANIZATIONS

National organizations for neutron scattering exist in Germany and Russia (committees), the UK (joint IOP/Royal Society of Chemistry group), and Italy and Switzerland (societies). There are plans to form a society in France, a society-based group in Austria, and an organization in Spain.

# **Full Professorship**

The Technical University of Denmark (DTU) invites applications for a full professorship associated Mikroelektronik Centret (MIC) in condensed matter opto-electronics.

The professor shall strenghten MIC's R&D programme within advanced semiconductor materials and their application in opto-electronic components and devices. Nonlinear ultrafast dynamics is of interest for optical switching as is the development of new technologies for the realisation of nanostructures for electronics, optics and mechanics. The successful candidate should document a profound knowledge of modern low-dimensional materials and their optical properties.

The professor is expected to contribute to the dynamical research environment at MIC and DTU. In addition to excellent professional skills, the professorship will therefore require flexibility and an ability to outline competitive research goals of relevance to external partners from industry and academia.

Within DTU, MIC is responsible for educating students in semiconductor process technology and microand nanotechnology. The professor will be responsible for supervising PhD students and giving graduate as well as advanced undergraduate lectures.

For further information, contact Director Ove Poulsen, Tel. +45 4593 4610 or Rector Hans Peter Jensen, Tel. +45 4588 2222. Applications should be sent to: Rector, Technical University of Denmark, Bldg. 101A, DK-2800 Lyngby, Denmark, before **Nov. 10th.** The successful candidate is selected by an expert committee refering to the Rector of DTU. Applicants will receive the results of the final expert evaluation. The evaluation will, however, not be published without approval of all applicants.



MIC is a new research centre at the Technical University of Denmark. Our research focuses on semiconductor-based technologies. Strong emphasis is on microsystems encompassing full integration between integrated optics, micro- and nanotechnology, and electronics. Major Danish industries work together at MIC. Our new process laboratory is in full operation and in addition MIC has established state-of-the-art photonics laboratories, including a new fs-laboratory.

The discussions to form a new organization to represent Europe's neutron scattering community come at a time when several international bodies are taking a fairly close look at future requirements. It is therefore perhaps natural that the community itself feels it needs to speak with a more coherent voice. Participants at the EPS Large Facilities in Physics Conference in Lausanne (12-14 September) heard of evaluations by the OECD Megascience Forum (its report will be published later this year) and by the European Union of Physics Research Organizations (EURPRO). UNESCO's Physics Advisory Council is making a general overview of facilities, the European Science Foundation is planning to examine neutron requirements, while the European Commission monitors neutron users fairly closely in the context of its Access to Large Installations initiative (which will continue in the 4th Framework programme 1994-98). The main issues are: The extent to which large facilities such as the ILL reactor source and the Rutherford-Appleton Laboratory's ISIS spallation source should be further developed. There is clear evidence that their full potential is unrealized and that any increase in support to allow increased access to neutrons would be used very efficiently as a relatively small proportion would need to be spent on fixed costs.

 The extent to which small, essentially national, centres should be involved in training specialists coming from many fields, improving detectors, and upgrading facilities.

 The importance attached to a major, new international source such as the proposed European Spallation Source providing a qualitative advance in performance that will take 10-20 years to realize.

## ESRF INAUGURATED

The European Synchrotron Radiation Facility (ESRF) was inaugurated on 30 September by representatives of the 12 contracting partners and over 400 guests. J. Fillon, France's Minister for Higher Education and Research, with negotiations to settle the additional host-state contributions to CERN's LHC project in mind, referred to the ESRF as well adapted to constructing a "scientific Europe" because it exemplified an approach that was not too formalised.

