

Computational physics

Kenneth Wilson — comparing today's particle colliders with the microscopes of Galileo's time.

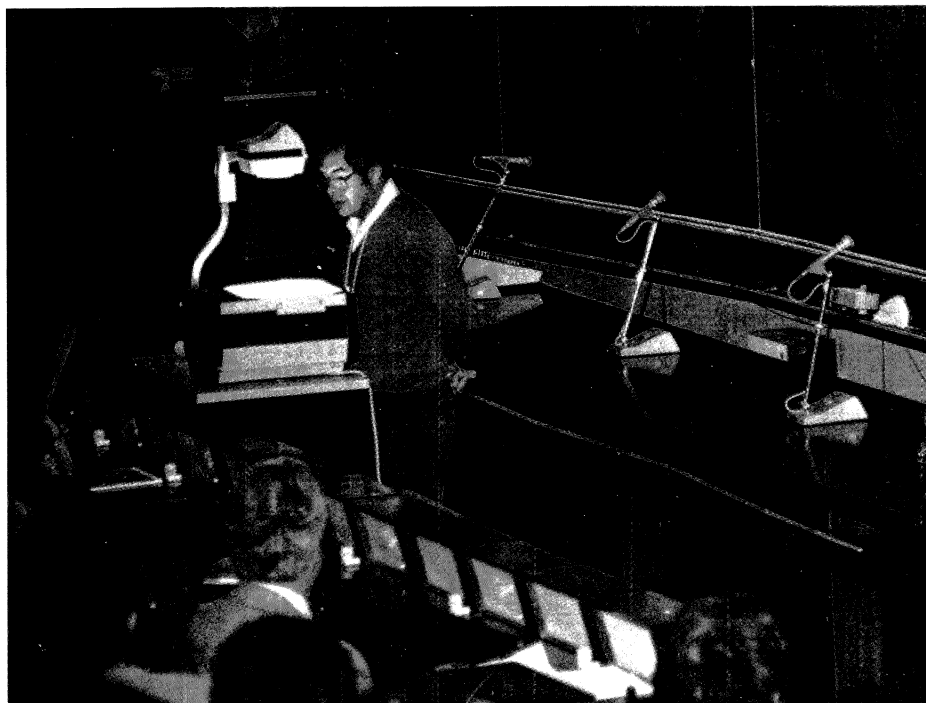
(Photo ICTP)

Computers have for many years played a vital role in the acquisition and treatment of experimental data, but they have more recently taken up a much more extended role in physics research. The numerical and algebraic calculations now performed on modern computers make it possible to explore consequences of basic theories in a way which goes beyond the limits of both analytic insight and experimental investigation.

This was brought out clearly at the Conference on Perspectives in Computational Physics, held at the International Centre for Theoretical Physics, Trieste, Italy, from 29-31 October. It was directed by Fred James (CERN), Alvis Nobile (Trieste), and Claudio Rebbi (Brookhaven and Boston).

The birth of computational physics can be traced back to the late 1960s with the first journals, conferences and schools on the subject. Although enormous progress has been made since then and whole new fields such as lattice gauge calculations have started up, it is clear that computational physics is still in its infancy. In fact Ken Wilson (Cornell) in his invited talk compared the current situation in computational physics with that of experimental physics at the time of Galileo when important discoveries were made using rudimentary microscopes, telescopes and leaning towers. Four hundred years later, experimental physics has developed techniques capable of penetrating many orders of magnitude deeper into matter and into the universe.

By analogy we expect that four hundred years from now it will be possible to perform calculations many of orders of magnitude more complex, and future computing engines compared with those of



today will be like today's particle colliders compared with the microscopes of Galileo's time.

For Wilson, perhaps the greatest algorithmic challenge facing contemporary computational physics is demonstrated by the problem of electronic structure. Here is an area where the basic theory, quantum electrodynamics, is known to be valid to an extremely high accuracy, sufficient to predict the physical, chemical, and biological properties of all atomic and molecular states. However current calculation techniques are barely powerful enough to compute gross properties of systems involving a few hundred electrons, with computing time increasing typically as the square of the number of electrons, and interesting chemistry and biology taking place in the region up to millions of electrons at least.

But the conference was not only devoted to dreaming about the future: world experts in many

areas of computational physics reviewed the state of the art from all points of view: physics algorithms, software techniques, and hardware developments, as well as their interrelationships.

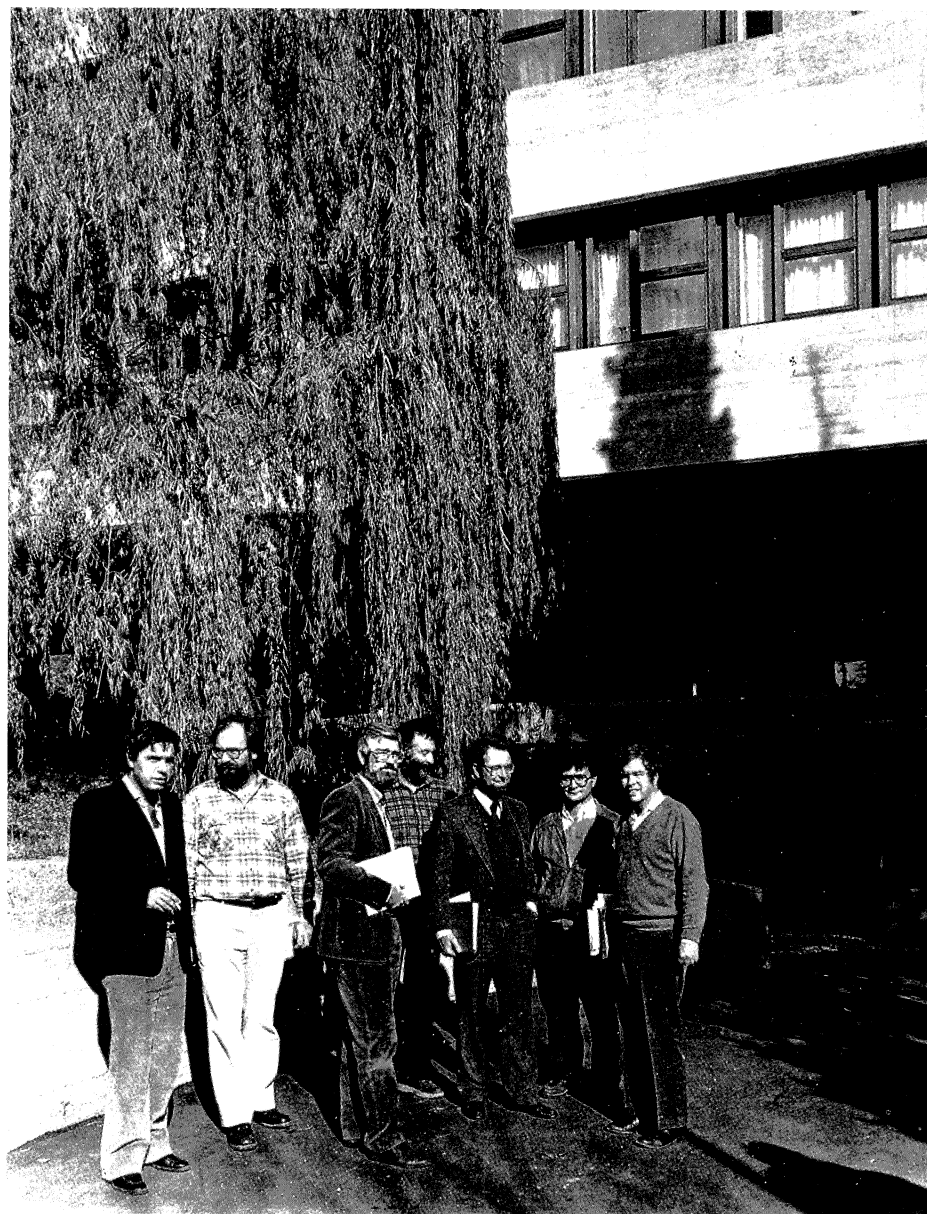
Supercomputer architecture was of course a topic of interest to all participants, and was covered in talks by several physicists and representatives of computer manufacturers. The physics areas covered in greatest detail, in addition to several aspects of electronic structure, were lattice gauge theory, stellar dynamics, and many-nucleon systems.

One of the highlights of the conference was the real-time demonstration of the possibilities of cellular automata by Tom Toffoli (MIT). In these discrete systems, each successive state is derived from the previous state by a relatively simple rule, which may be deterministic or partly random. By varying the replication rule, Tom

was able to model many mathematical and physical phenomena from shock waves to fractal growth and stellar dynamics. Using his own special hardware board under the control of an Olivetti M24 personal computer he was able to calculate successive states of the automata with sufficient speed that large-screen colour projection gave an uncanny feeling of observing the evolution of complex continuous systems obeying known 'physical' laws. This provides considerable insight into important phenomena like order and disorder, phase transitions, stability and reversibility in physical systems.

The conference took place immediately after the School on Advanced Techniques in Computing in Physics, held also at ICTP and with the same organizers. The three-week school offered in-depth courses on pure computing topics (programming languages, operating systems, networking, etc.), numerical and symbolic analysis techniques, and physics applications, to 150 students selected from over 400 applicants, and coming mostly from the developing countries.

These 'students' turned out to be highly qualified computational scientists, which made for an unexpectedly lively and stimulating school. One of the lecturers even remarked that it was his most responsive audience, despite having given similar talks as seminars in some of the world's most prestigious laboratories. One explanation was the school's highly selective acceptance procedure, but it is also a clear sign that competence in computing is increasing fast in many less developed countries. Only a few years ago, access to a reasonable computer meant the



installation of an entire computer centre, with everything from a false floor to a team of systems analysts, all of which was beyond the possibilities of many countries. Nowadays the same computer power is available just by plugging in a PC. The effects of this quiet revolution have been spectacular.

Most of the 150 school participants stayed on for the conference, where they were joined by

At the Conference on Perspectives in Computational Physics held at the International Centre for Theoretical Physics, Trieste, Italy, in October. Left to right: G. Parisi, A. Nobile, F. James, G. Jacucci, C. Rebbi, T. Toffoli and K. Wilson.

(Photo G. Montenero)

about 70 more people (nearly all from Western Europe and North America).

One evening was devoted to an open discussion of the future of Computational Physics. The presence of large delegations from developing countries made it a natural forum for computational physics research in the poorer regions of the globe. One western participant said he had never be-



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fore been at a conference where so many developing countries had been represented, and it clearly came as a surprise to him and others that it was not only possible to carry on computational physics research in such places, but that it was being done actively. The obvious conclusion is that this enormous source of intellectual potential cannot be neglected.

Ken Wilson's summary talk covered the major outstanding issues for computational science as he saw them and as they were brought out at the conference. His first point was: what is quality research? Or, equivalently, what research will still be respected four centuries from now?

The great algorithmic challenges remain: electronic structure (solu-

tion of the Schrödinger equation), turbulence, function minimization (for protein folding, spin glasses, etc.), quantum field theory, and stellar evolution. The difference in the time-, length-, and energy-scales is impressive.

Communications issues are also very important. The usual language of Computational Physics, Fortran, has long been recognized as inadequate in many respects, especially as a vehicle for explaining what a program is expected to do. Yet none of the many other languages has had widespread acceptance.

There are other important aspects of the publication issue: Where should new papers be published, where and how should programs be published? The list of journals needed for a complete

Computational Physics library is enormous. And there is networking, which both solves and introduces many problems, but does not obviate the need for centres of excellence.

The economic aspects of the research cannot be neglected. The future of Computational Physics will depend on how we interact with the larger scientific computing market, which has a huge industrial base representing about \$ 10 billion per year, and is truly international. With the technology advancing rapidly on many fronts, the prospects for Computational Physics are apparently limited only by our own skill and imagination.

By Fred James

At the 'Jackfest' marking the 65th birthday of Jack Steinberger (see July/August 1986 issue, page 29), T. D. Lee gave an account of the history of the weak interactions. Lee was a graduate student with Steinberger under Enrico Fermi in Chicago from 1946, and went on to win the 1957 Nobel Physics Prize with C. N. Yang for their suggestion that the weak interaction does not conserve parity (mirror symmetry). This edited version omits some of Lee's tributes to Steinberger, but retains the impressive insight into the subtleties of a key area of modern physics by one who played a vital role in its development.*

* The full version is available as a 'Yellow Report' No. 86-07 from CERN Scientific Information Service.

History of the weak interactions

by T. D. Lee

In 1898 Rutherford discovered that the so-called Becquerel ray actually consisted of two distinct types of radiation: one that is readily absorbed which he called alpha radiation, and another of a more penetrating character which he called beta radiation. Then, in 1900, the Curies measured the electric charge of the beta particle and found it to be negative. That, at the turn of the century, began the history of the weak nuclear interaction. From the very start the road of discovery was tortuous, and the competition intense.

A letter written by Rutherford to his mother expressed the spirit of research at that time: 'I have to keep going, as there are always

people on my track. I have to publish my present work as rapidly as possible in order to keep in the race. The best sprinters in this road of investigation are Becquerel and the Curies...' Rutherford's predicament is very much shared by us to this day.

Soon even more runners appeared: Otto Hahn, Lise Meitner, William Wilson, von Baeyer, John Chadwick, Niels Bohr, Wolfgang Pauli, Enrico Fermi, Charles Ellis, George Uhlenbeck, and many others. We know that to reach where we are today took nearly a whole century and a large cast of illustrious physicists. Yet probably any modern physicist is only three handshakes away from these pio-