Focussing on the Science

Ralf Gruber, who co-chaired PC'94 with Marco Tomassini, describes the issues modern computational physics aims to address.

Ralf Gruber and Innes Buzzini Soldati at PC'94.

PC'94 — the biennial EPS-APS conference organized every other year in Europe by the EPS Interdivisional Group for Computational Physics — dealt with numerical experiments that simulate real ones which would be too big, too small, too hot, too dangerous, too rapid, too slow, or too costly. One of the major themes was to bring together specialists from different research domains so that they could exchange old and new ideas and learn from methods developed in different fields of computational physics, but use similar methods.

Overlapping Fields

Many models and algorithms that have been initiated in a specific domain have later on been reused in other fields. For example, particle pushing is now applied in computational fluid dynamics, plasma physics, astrophysics, meteorology, and material sciences; Poisson solvers are applied to problems in electrodynamics, diffusion, fluid mechanics, casting, or to create an adaptive mesh.

The simulation of a realistic industrial problem now makes use of methods coming from several different fields. Hence, the optimization of an industrial laser requires the application of models in thermodynamics, structural analysis, and optics; numerical experimentation for chemical reactors combines Navier-Stokes flow with thermodynamics, molecular dynamics, particle simulation, and structural analysis. For complex geometries, computer-assisted designs must be integrated in the simulation process, but we still do not know how to do this efficiently.

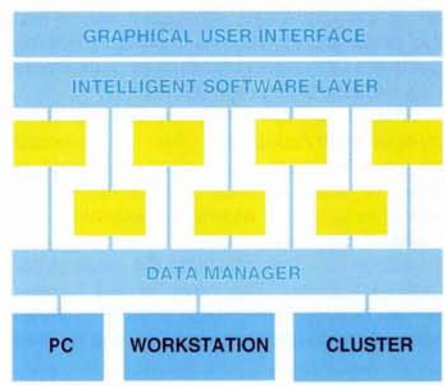
New models must sometimes be combined with established ones. For instance, to simulate an electrofilter that eliminates polluting particles from a gas, well-known models are applied to simulate the electrodynamics, particle tracking, and the current and charge density distributions. However, new models need to be developed and validated using real experiments for the ionization processes in the corona region, and for the deposition of the pollutant particles at the filter wall. All the interdependent variables have to be integrated in a self-consistent manner.

Our approach to solving problems is changing with the increase in the power of computers. We are making the physics more complete and increasing the complexity of our models; we are discovering new iterative numerical algorithms with improved convergence properties that have to be adapted to the many new computer architectures appearing on the market.

Beside these modelling and algorithmic matters, a computational physicist has to struggle with implementation problems. One has to worry about vectorization, parallelization, data structures, data flow, visualization, archiving, and even user interfaces. How can we handle all this without becoming a computer scientist? The task of a physicist, chemist or an engineer should be to solve a scientific problem without caring so much about parallel computer architectures, data management systems, three-dimensional data visualization, nor about how to combine different application programs to solve an interdisciplinary problem. There are very competent applied computer scientists now who can do this work much more effectively.

The Scientific Macintosh

New systems called program environments have to be developed and standardized. They should offer the integration functionalities needed to solve interdisciplinary problems including a data manager, a visualization system, a data monitor to access data all the time, a graphical user interface through which the physicist can adequately define a problem, and an intelligent software layer to help a user carry out pre- and post-processing and to execute his modules on the most appropriate computing configuration. The user should be able to computer simulate in the same way as a secretary edits letters. It should not be necessary to be concerned with particular computer platforms (indeed, this is a necessary condition for the acceptance of massively parallel machines by pragmatic users). The user would in effect like to benefit from a "scientific Macintosh" that aims to bring supercomputing power to a person's desk. The illustration demonstrates one of the first prototypes of a programming environment of this type.



The scientific Macintosh envisages a user-support environment for easily accessing a wide variety of computational packages via a uniform graphical user interface. It is based on a common database, well-defined data exchange and an integrated visualization system. The applications are ported and optimized on heterogenous hardware so that the optimum computer architecture for a given simulation can be established. The user need only learn one set of input and visualization procedures regardless of the application, and can always access the most advanced system. The illustration represents the PECCAM environment for computational chemistry and materials science which is being developed by the Swiss Scientific Computing Centre. A data carrier (in blue) enables the flow of data to users, applications and various computers via a user interface, a software layer to guide execution of computational modules, a control system, and a distributed data manager. Application packages (in yellow) to calculate, for instance, electronic structure and to carry out molecular dynamics and other types of simulations are embedded in the PECCAM environment.

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Some 230 scientists from 13 countries attended the 6th Joint EPS-APS International Conference on Physics Computing (PC'94), organized by the Centro Svizzero di Calcolo Scientifico (CSCS) of the Swiss Federal Institute of Technology, Zurich (ETHZ). The scientific advisory committee chaired by Ralf Gruber did an excellent job in putting together an attractive programme, and the reading committee guaranteed a high scientific level for the conference and the proceedings (which were available at the conference). Thanks go to the Swiss PTT, Fritz Hille and especially to Silvia Giordano who were able with their groups from the CSCS and the ETHZ to have a local-area network running in time. Angelo Mangili, Marco Tomassini and Ines Buzzini Soldati handled most of the organization. Jörg Heiniger from the ETHZ helped greatly in organizing the very successful industrial exhibition. The highlight of the accompanying programme was a concert that featured three extremely gifted young soloists accompanied by an orchestra directed by a famous Swiss conductor.

PC'94 was helped considerably by sponsors, notably Swissair and Crossair who offered free tickets to invited speakers, the town of Lugano and Ente Turistico for entertainment, Convex, NEC, Sun, CSCS, Musica Ticinensis, Rete2, Radiotelevisione di Lingua Italiana, and SMR for support of various types, the Swiss National Science Foundation and the International Science Foundation for funds to allow scientists from east and central Europe to attend, and *Computer in Physics* for the programme. Several commercial exhibitors contributed actively by presenting their products.

The proceedings, published by EPS (730 pages; price: SFR 100.–), can be ordered from Mrs. I. Buzzini Soldati, CSCS, Galleria 2, Via Cantonale, CH-6928 Manno, Switzerland; fax: +41-91-50 67 11; pc94@cscs.ch.