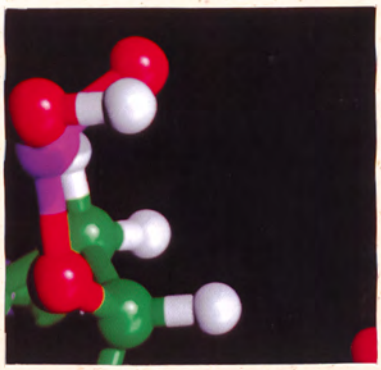
A N N U A L · R E P O R T

Centro Svizzero di Calcolo Scientifico

C S C S

Swiss Scientific Computing Center



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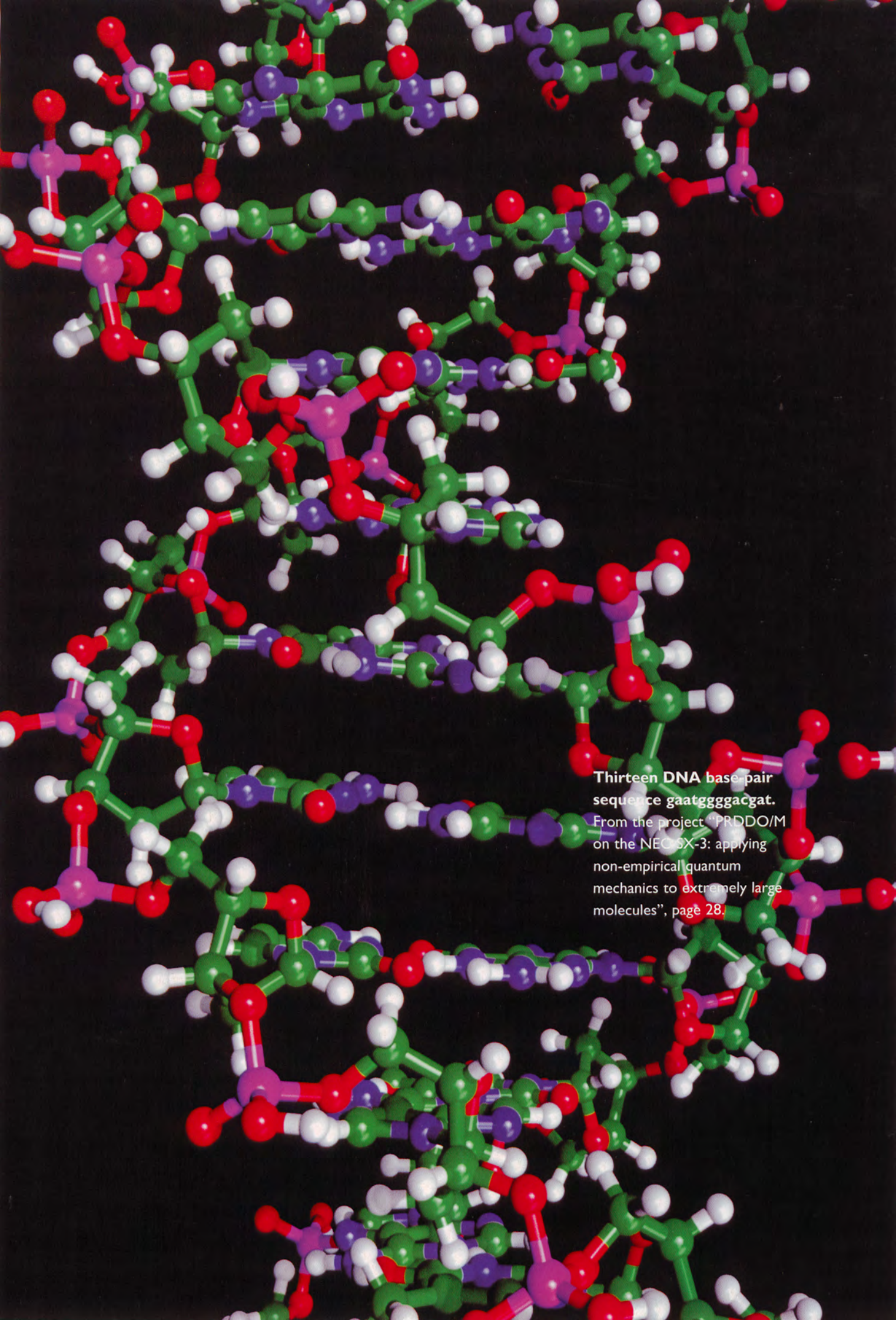
ETH Eidgenössische Technische Hochschule Zürich
Ecole Polytechnique Fédérale de Zurich
Politecnico federale di Zurigo
Swiss Federal Institute of Technology Zurich



Thirteen DNA base-pair sequence gaatggggacgat. From the project "PRDDO/M on the NEC SX-3: applying non-empirical quantum mechanics to extremely large molecules", page 28.

Centro Svizzero di Calcolo Scientifico (CSCS), also known as
Swiss Scientific Computing Center, is affiliated with the
Eidgenössische Technische Hochschule Zürich (ETHZ), also
known as the Swiss Federal Institute of Technology Zurich.

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Bronze "portable"

Roman abacus,

beginning of

Christian Era.

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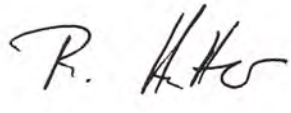
PREFACE

The speed of change in our world is accelerating and new challenges to our lives, our society and our environment are appearing fast. New social paradigms, rapid market globalization, new infectious diseases and climate change exemplify this development. Discovery of the first antibiotic took mankind thousands of years—finding the key to change the genetic information of our world's beings took only another 30 years! Our most urgent challenge, and central for the well-being of our planet, is finding the transition from quantitative to qualitative behavior to guarantee sustained development. Emerging technologies can support this effort.

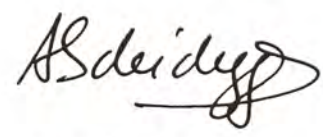
High-performance computing (HPC) is such an emerging technology, a technology which can exert a tremendous influence in the problem-solving process. For the last two decades, HPC has been successfully applied to push the limits of our scientific knowledge. We now see HPC moving into industry and impacting product life cycle activities. In the near future, HPC will be mandatory in our efforts to cope with the big challenges of mankind.

But HPC in itself has many challenges. The technology leap from a single (or few) processor architecture to one with thousands of processors is complex and difficult; such a leap requires new paradigms in software development and will probably occupy software developers and application specialists for another decade. Geographically distributed and decentralized computing and data resources require an altogether new dimension of data transfer capabilities—new problems that still must be solved. And finally, the move of HPC from the halls of science to a commercial, user-friendly, general purpose tool presents us with another significant challenge. Only by mastering the leap into another magnitude of performance and by commercializing user-friendly applications can we hope that HPC will play the important role it deserves—supporting our problem-solving processes to resolve our most difficult challenges and tasks.

We hope that CSCS, and other HPC application centers, will continue to gain significance and participate decisively in shaping our future. We have to welcome and be prepared for the integration of HPC into our lives; we have to educate our society for acceptance—and to qualitatively explore the quantitative possibilities that HPC offers us. Because finally, it is not the machine that will reveal the solution but enlightened human beings with intelligence and compassion.



Prof. Dr. Ralf Hütter
Vice-president Research ETHZ



Dr. Alfred Scheidegger
Director CSCS

Expert calculating on a token abacus, XVI Century.

The Swiss Scientific Computing Center is the national high-performance computing center. Its mission is to serve the scientific and economic community with state-of-the-art computing facilities, expert human resources and user support. In 1994 CSCS experienced a remarkable growth in regard to the computing facilities as well as human resources and project acquisition. The year was characterized by three major activities: the enhancement of user support and services, the expansion of cooperative research with particular focus on industrial collaboration, and the extension of educational and regional activities.

User Support and Services

The user support entity, with the Help Desk as CSCS's point-of-contact, was restructured to enhance information flow from and to users. Continued effort was put into user code optimization with the objective to maximize the cost-effective utilization of the computer facilities. Computation resources are evaluated to target the most appropriate platform for the user and the desired application software, with improved performance as the result. Support for visualization was in high demand, providing users with many images and videos of their project results; new activities in tele-conferencing and tele-working saw initial sessions.

The users can profit from the considerable upgrade in computing power and the introduction of new software: the installation of an 8-processor Convex Meta workstation cluster (1.55 GFLOPS), a 6-processor Convex Exemplar (1.17 GFLOPS), and a 128-processor NEC Cenju-3 (6.4 GFLOPS) parallel machine for pilot usage. New services in high-performance data transmission are now available through an ATM-network pilot project of the Swiss TELECOM PTT. And finally, the data-link to the Joint Research Centre of the European Union in Ispra (Italy) was augmented to 512 Kbit/s.

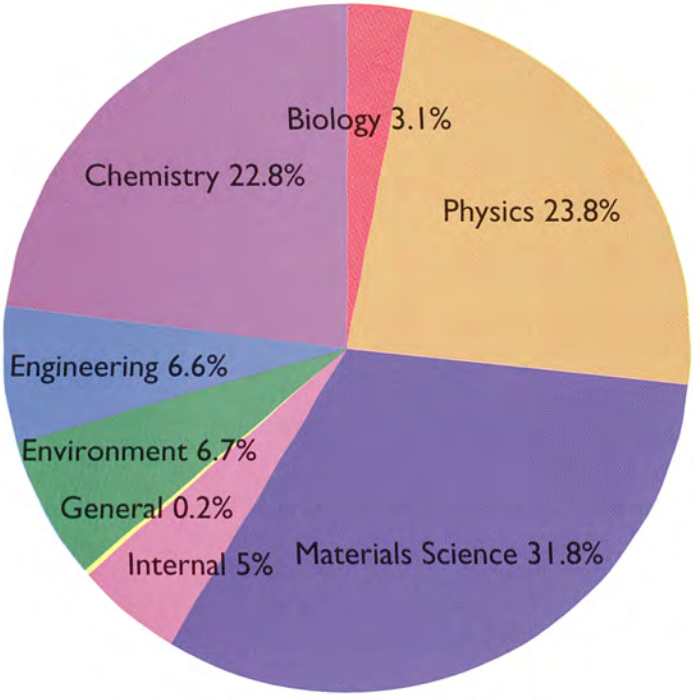
The primary application fields on CSCS computing machines in 1994 were: materials science, physics, chemistry, engineering, and climate studies. CSCS users are still predominantly academic users, as can be seen in the next pages.

Collaborative Research Projects

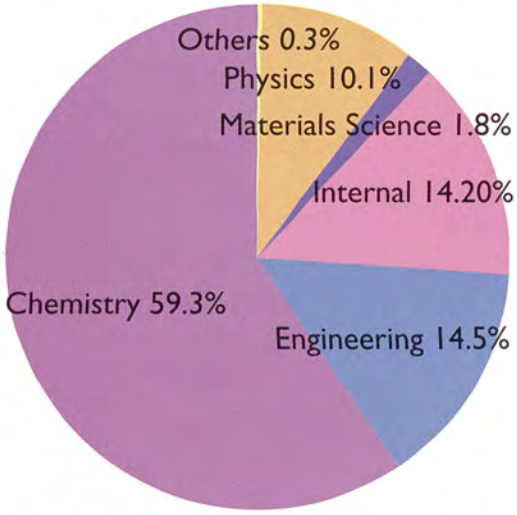
Collaboration between industry and academic institutions brings direct benefit to both partners and indirectly to society as a whole. CSCS is committed to continuing and initiating collaborative research projects in significant impact areas. Third-party funds supporting such projects totaled 2.5 million Swiss francs in 1994.

Swiss industry, while heavily involved in workstation computing, is still relatively conservative in its use of high-performance computers; interest, however, has increased dramatically. This is reflected by industry's increased willingness to enter into collaboration with CSCS and to take advantage of existing expertise. In 1994, CSCS successfully concluded several collaborative industrial projects and commenced various new initiatives under the Industrial Partnership Program. Aside from contracts with big industry (like ABB, Agusta, Ciba, Convex, Cray, NEC, and Electricité de France), several small- and medium-sized enterprises established collaborative contracts with CSCS. The Joint CSCS-ETH/NEC Collaboration in Parallel Processing, employing eleven researchers, was extended until 1996.

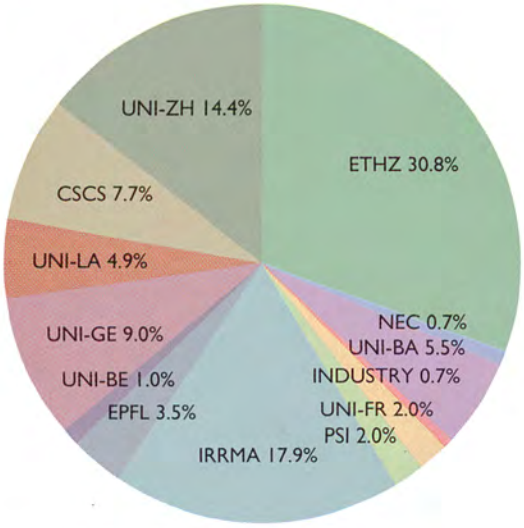
Collaborative research and development projects with European organizations and other academic institutions were concluded and others newly launched; the initiation of a pilot project for a national remote sensing image archiving is considered an important step towards national resource coordination. These collaborations are described in greater detail in the Research Projects section, *page 17.*



NEC SX-3, 1994 CPU usage by field.



HP Workstation Cluster, 1994 CPU usage by field.



NEC SX-3 + HP Workstation Cluster, 1994 CPU usage by organization.

LARGE USER PROJECTS

User projects at CSCS cover a wide range of application fields and represent diverse disciplines from all Swiss universities and federal institutes of technology. The following is a list of the 1994 large user projects, each of which requested more than 10CPU hours per month on one processor of CSCS' NEC SX-3.

Astrophysics

Nussbaumer, Prof. H.–Institut für Astronomie, ETHZ: *Zusammenstossende Sternwinde in Symbiotischen Doppelsternsystemen.*

Biology

Braun, PD Dr. W.–Institut für Molekularbiologie und Biophysik, ETHZ: *Struktur und Dynamik von Proteinen.*

Chemistry

Daul, Dr. C.–Institut de Chimie Inorganique et Analytique, Université de Fribourg: *Computational coordination chemistry.*

Huber, Prof. H.–Institut für Physikalische Chemie, Universität Basel: Ab-initio *Berechnung zwischenmolekularer Wechselwirkungen und deren Verwendung in Simulationen von Flüssigkeiten.*

Leutwyler, Prof. S.–Institut für anorganische, analytische und physikalische Chemie, Universität Bern: *Electronic structure and vibrational calculations of hydrogen-bonded clusters.*

Mareda, Dr. J.–Département de Chimie Organique, Université de Genève: *Quantum chemical studies of reactive intermediates and mechanisms of organic reactions.*

Quack, Prof. M.–Laboratorium für Physikalische Chemie, ETHZ: *Spectroscopy and dynamics of molecules and clusters.*

Thiel, Prof. W.–Organisch-Chemisches Institut, Universität Zürich: *Quantenchemische Berechnung von Potentialflächen.*

Weber, Prof. J.–Département de Chimie Physique, Université de Genève: *Quantum molecular modeling of catalysts; Structure and electronic properties of elemental and chemisorbed semiconductor surfaces.*

Engineering

Eberle, Prof. M.K.–Institut für Energietechnik, ETHZ: *Computation of unsteady three-dimensional flows in complex geometries.*

Rys, Prof. F.–Laboratorium für Technische Chemie, ETHZ: *Teilchenwachstum in laminarer Flüssigkeitsströmung.*

Environment

Beniston, Dr. M.–Geographisches Institut, ETHZ: *High resolution climate simulations; Simulations of the influence of the Alps on climate; Simulations of the ozone layer depletion; Ray tracing model development.*

*Olivier, Prof. R.–Institut de géologie, UNIL: *Traitement des données sismiques de réflexion dans le cadre de l'étude géologique du soubassement alpin.*

*Stocker, Prof. T.–Physikalisches Institut, Universität Bern: *Ocean and climate; Modelling the biogeochemical cycle of carbon.*

*Zuur, Dr. E.–Institut de géologie, Université de Neuchâtel: *Limnoceane.*

Materials Science

Baratoff, Dr. A.–Institut für Physik, Universität Basel: *Ab initio simulations of surfaces and scanning probe microscopies.*

Car, Prof. R.–IRRMA-EPFL: *Quantum Simulation of Materials.*

Jarlborg, Dr. T.–Département de Physique de la matière condensée, Université de Genève: *Elastic and dynamical properties of solids; Heavy fermions; Study of high Tc compounds; Electronic structure of disordered materials.*

*Maric, Dr. D.–CSCS: *Program environment for computational chemistry and materials science.*

Massobrio, Dr. C.–Institut de Physique Expérimentale, EPFL: *Numerical simulation of clusters deposition on surfaces.*

Suter, Prof. U.–Institut für Polymere, ETHZ: *Monte Carlo-Simulationen von Polymeren.*

Physics

Appert, Dr. K.–CRPP-EPFL: *Propagation d'ondes dans un plasma chaud torique axisymétrique.*

Cooper, Dr. W.A.–CRPP-EPFL: *Computation of stellerator coils, equilibrium and stability.*

*Durrer, Prof.R.–Physik Institut, Universität Zürich: *Cosmological structure formation with topological defects.*

Jegerlehner, Dr. F.–PSI: *Monte Carlo simulation of weak bosons as composite particles.*

Meier, Prof. P.F.–Physik Institut, Universität Zürich: *Berechnung der elektronischen Struktur von Störstellen in Festkörpern; Quantum Monte Carlo Investigation of Correlated Electron Systems.*

Moullet, Dr. I.–Section de Physique, Université de Lausanne: *Study of Aluminium clusters deposited on surfaces; Study of transition metal liquid.*

Rice, Prof. T.M. and PD Dr. D. Würtz–Institut für Theoretische Physik, ETHZ: *Numerische Verfahren zur Simulation stark wechselwirkender fermionischer und bosonischer Systeme.*

* New Project

Educational Activities

CSCS's educational and local outreach activities range from highly-specialized training to general computer education sessions.

CSCS's Education Laboratory (EdLab) provides a framework for teaching and training in the fields of applied computer and computational sciences, and its goal is to transfer such knowledge into education, services and industrial products. The fields cover novel computer architectures, novel software systems, scientific computing, non-numerical computing, and software engineering.

The Summer Student Internship Program (SSIP) was conducted for the second time; the program, which focusses on teaching parallel computing and on the involvement into short research projects, brought together ten gifted undergraduate students from eight different countries around the world.

For local outreach, the Education Program for Schools was established as a result of a common effort with the government of the Canton of Ticino. The goal is to promote applied computing and communications (systems) for applied science for different school levels. The program is comprised of three activities: school visits for middle schools, the development of curricula for integration into the respective teaching fields, and the computing and communications camp (the C^3 Program) for highly-skilled, pre-college students.

Finance and Personnel

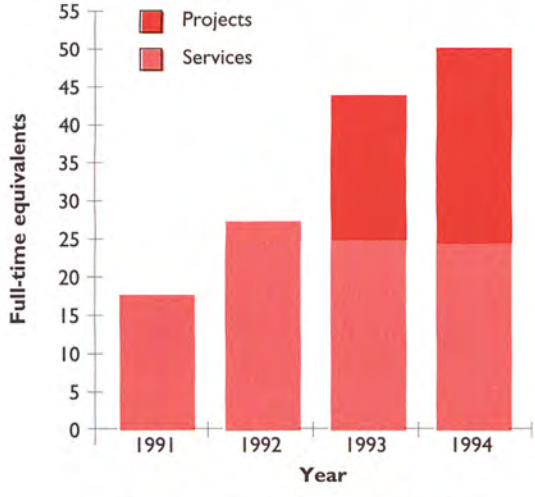
The financial development of CSCS was marked by an increase of 14% in personnel expenditure for services to the national users and of 18% in acquired project-related third-party funds. In addition to the federal funds for operations and personnel (shown in the graph, page 11), 2.4 million SFr.

Moments from the SSIP'94.

	Federal Funds (KSFr.)			Third-party Funds (KSFr.)		
	1992	1993	1994	1992	1993	1994
Personnel	1,435	1,932	2,318	449	1,198	1,681
General Expenses	512	556	582	641	678	537
Total Expenses	1,947	2,488	2,900	1,090	1,876	2,218
Federal Contribution	1,947	2,488	2,900			
Income				928	2,011	2,451
Result	0	0	0	-162	135	233
Third-party Funds						
Reserves/Contributions	31.12.1992			1,597		
	31.12.1993				1,732	
	31.12.1994					1,965
Increase 1993					135	
Increase 1994						233

were invested for hardware, software and networking installations. Costs for computing infrastructure maintenance, physical infrastructure (such as the building and maintenance), and for the utilization of the wide area networking are covered under the financial aspects of ETH Zürich.

The increase in third-party funding, totalling about 2.5 million SFr., is a result of the numerous collaborative research and development projects acquired in 1994; half of this funding was contributed by private industry. This increase in project activity spurred personnel recruitment with the result that CSCS staffed 50.25 full-time equivalents by the end of 1994 (an increase of 12% above 1993).



1994: Personnel full-time equivalents in Services (24.5) + Projects (25.75) = 50.25 full-time equivalents.

Future Outlook

CSCS is moving in the direction of optimized high-performance computing with emphasis on cost-performance ratios and user-friendly environments and tools. We recognize that to offer good user service it is critical to enhance coordination and integration of knowledge and software, nurtured by the various research and development results and the experience gained in the numerous application fields. Such a service forms also the basis for absorbing the increased interest of industry to collaborate with CSCS. The optimal structure lies in a nation-wide distributed computing system, to which CSCS is committed.

CSCS is dedicated to the education of its users and the next generation of computer users. Programs for children and young adults will play an increasing role in CSCS's education activities—with the realization, of course, that the machine can do no better than the human being who pilots its power.

Manual Counting, from "Theatrum Arithmetico-Geometricum" by J. Leupold, 1727.

While 1993 had been a year of major changes in the configuration of CSCS and its service, 1994 focused on the further development of these resources: stabilization, tuning, and expansion.

Vector Power

The NEC SX-3/24R is CSCS's main vector computing resource, configured with two processors, each one having 16 pipelines. The system delivers a peak performance of 12.8 GFLOPS at a clock cycle of 2.5 ns. The SX-3 is equipped with 2 Gbytes of main memory and 4 Gbytes of extended memory. A new HiPPI-attached, 50 Gbytes Maximum Strategy RAID unit was added for scratch space.

Scalar and Parallel Power

In the first quarter of 1994, the high-performance workstation cluster (Convex Meta Series) was made available to users. This system is suitable for more scalar applications or for those users who want to develop parallel applications using PVM. Due to increasing demand, this scalar system was expanded by a 6-node parallel computer (Convex Exemplar), which is suitable for running sequential code and allowing users to move smoothly into parallel processing technology.

Three other parallel machines are available at CSCS: a NEC Cenju-3, a NEC Cenju-2 and a Meiko CS-1/860. The NEC Cenju-3 was installed at CSCS in the third quarter of 1994, and is configured with 128 processing nodes each with 64 Mbytes main dynamic memory. The system's basic purpose is to serve as a development platform for the Joint CSCS-ETH/NEC Collaboration in Parallel Processing. Besides that, the machine is open for pilot users to test and make suggestions for functionality enhancements of the tool environment Annai under development in the joint CSCS-ETH/NEC collaboration. Also available is the 16-processor Cenju-2 with 1024 Mbytes of memory, and the Meiko Computing Surface CS-1/860 with eight nodes each with 8 Mbytes of memory.

Software

CSCS offers a diverse set of application software and software tools in a variety of application fields (see table next page). In addition to widely used commercial software programs, a program environment is available for chemistry applications that assists in automatically distributing different tasks to the most suited machines to maximize the efficient usage of the CSCS computer facilities. A similar software environment is offered in the area of computational engineering. Other software is installed upon request.

Software available on the parallel platforms comprises a variety of compilers, different message-passing libraries such as CSTools, the Message-passing Interface standard MPI, and PVM, the Linda coordination language, and the powerful integrated parallel programming environment, Annai.

Visualization Laboratory

CSCS's visualization laboratory provides the high-quality facilities needed for visualization, video animation and editing, and color reproduction. A variety of powerful Silicon Graphics servers and workstations are accessible in the laboratory for high-performance, interactive three-dimensional rendering, for developing and tuning graphics applications and for medium-range visualization projects. General purpose software such as the modular AVS or Iris Explorer is used for visualization projects in most cases. Custom modules are often written to enhance the functionality and match the specific needs of the users.

Convex 3820 and Maximum Strategy RAID disk.

Storage Tek silos for archiving of large amounts of data.

NEC Cenju-3, 128-processor parallel computer.

MATHEMATICAL LIBRARIES

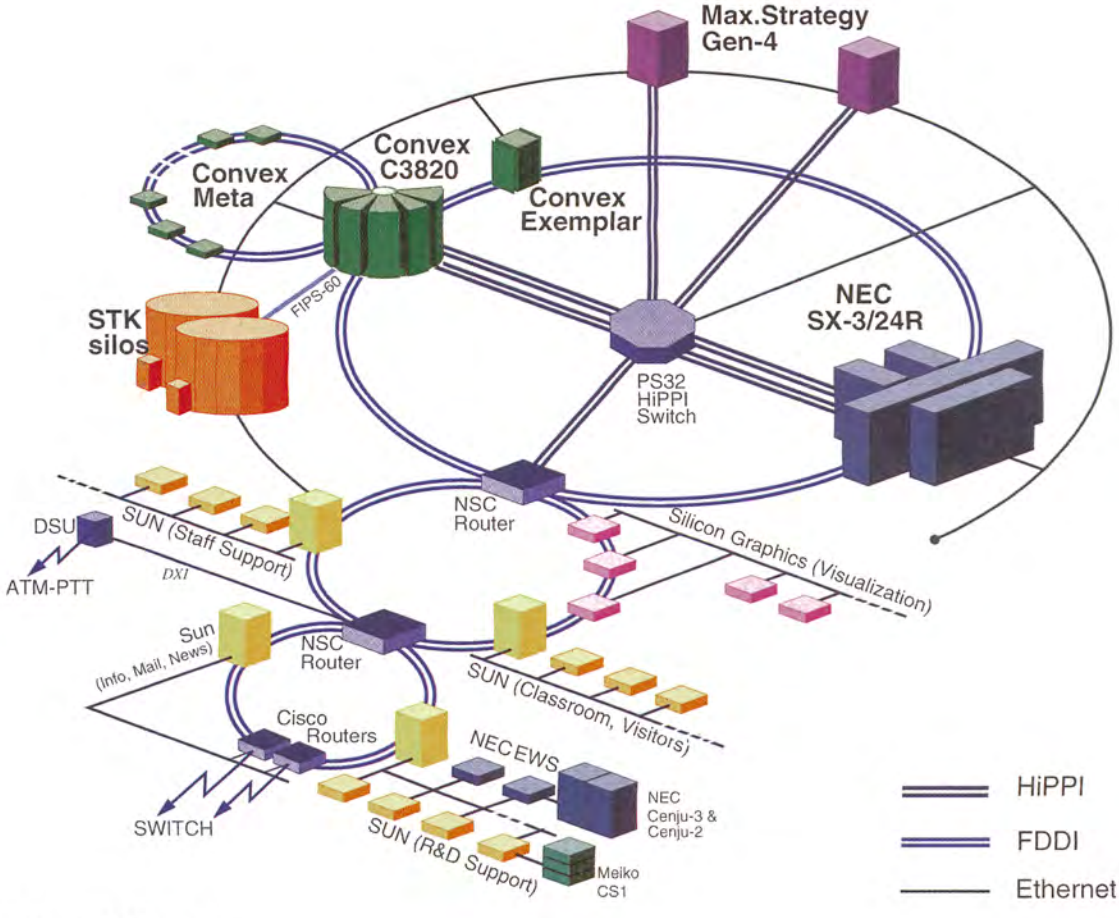
ASL ----------Advanced Scientific Library from NEC
BLAS ----------Basic Linear Algebra Subprograms, Levels 1, 2 and 3
EISPACK ----------Matrix Eigenvalue Problem Solver
LAPACK ----------Linear Algebra Routines Successor to Linpack and Eispack
LINPACK ----------Linear Algebra Subroutine Library
Maple ----------Symbolic Mathematics/Visualization
Mathematica ----------Symbolic Mathematics/ Visualization
MATHLIB ----------NEC Mathematical Library
Matlab----------"Matrix Laboratory" for Interactive Scientific Computation/Visualization
MINPACK ----------Non Linear Optimisation Package
NAG ----------General Mathematical Library

SCIENTIFIC APPLICATION SOFTWARE

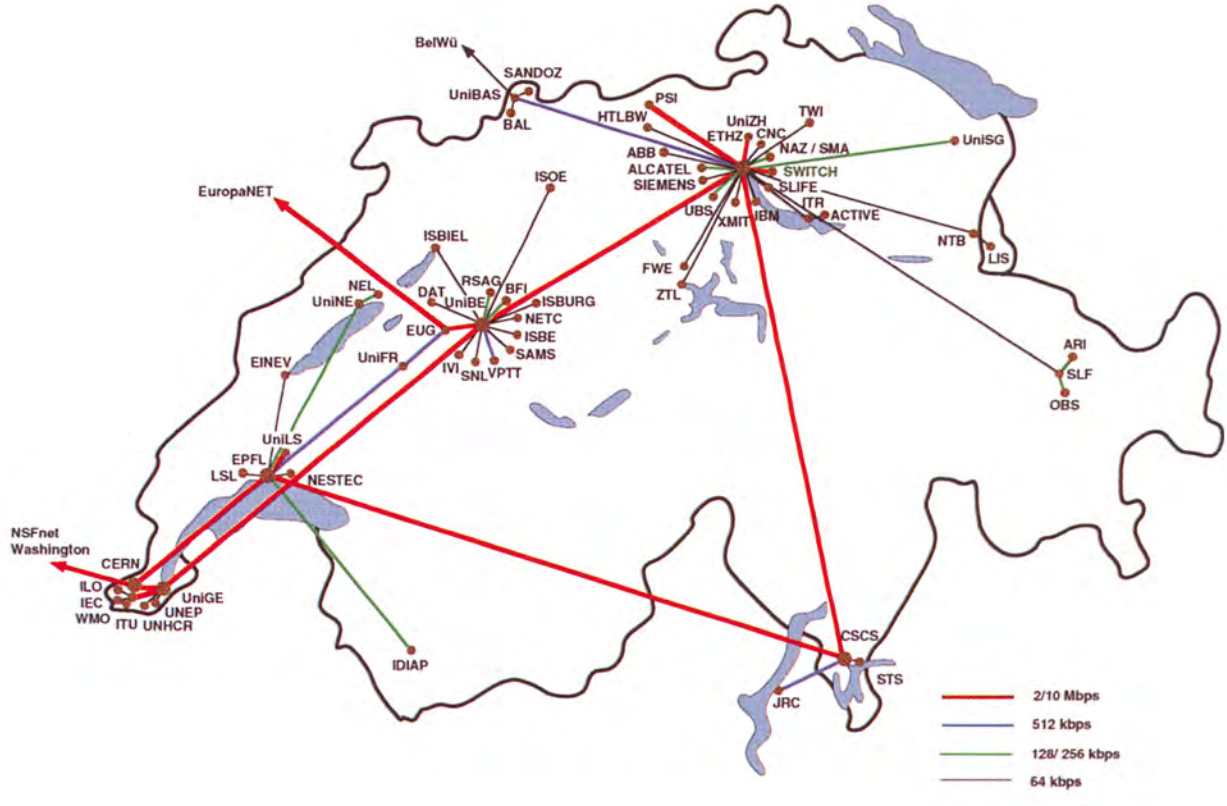
AMBER ----------Computational Chemistry
AMOSS ----------Computational Chemistry
B2000 ----------Finite Element Analysis
FLUENT ----------3-D Computational Fluid Dynamics Package
GAMESS-US ----------Computational Chemistry
Gaussian 92/DFT -----Computational Chemistry/Physics
Geomesh----------Computational Fluid Dynamics
HFSS ----------High Freq. Structure Simulation, Materials Science
LS DYNA 3-D---------Mechanical Engineering
MSC/NASTRAN------Finite Element Analysis Program
PE²AR ----------Engineering
TASCFLOW ----------3-D Computational Fluid Dynamics Package

VISUALIZATION

AVS----------Interactive Modular Visualization Package
AVS/Animator---------Additional Modules for AVS to produce animations
BASPL----------Engineering Visualization Software
IRIS EXPLORER ------Interactive Modular Visualization Package
MOLEKEL----------Molecular Graphics Package
MOSS ----------Civil Engineering Package
PV-WAVE----------Command Language Based Visualization Software
Video----------Video Preview and Recording Tool
Wavefront ----------Advanced Visualizer and Professional Composer



CSCS Internal Network.



SWITCH - Swiss Academic and Research Network. ©1994 SWITCH

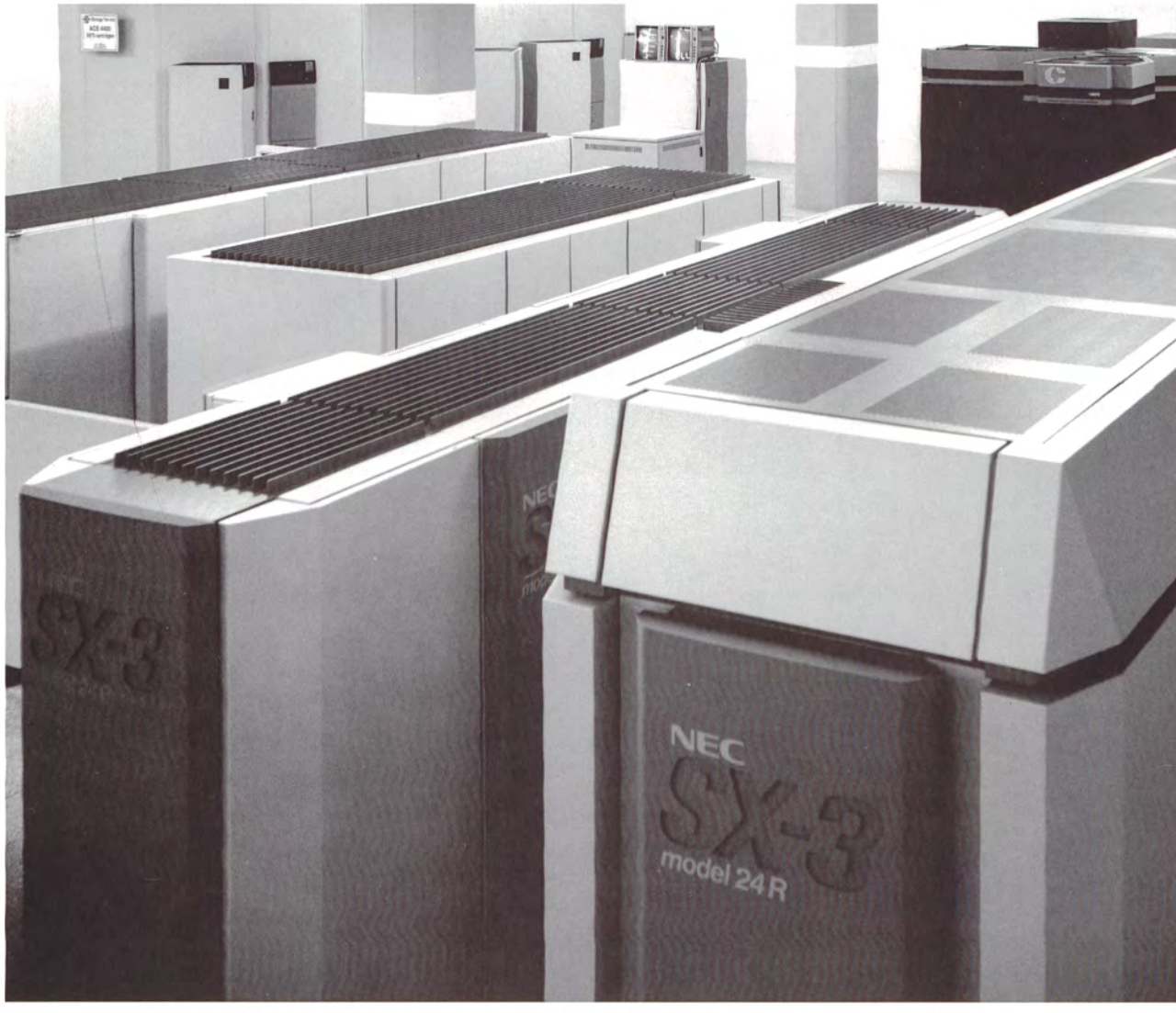
File Serving and Archiving

The two-processor Convex 3820 front-end system is equipped with 1 Gbyte of main memory and 60 Gbytes RAID disk space for users; the system runs UniTree, a hierarchical mass storage system. The Convex is not only the CSCS file and archive server, but also distributes batch jobs to the appropriate computing resources and serves as the interactive workplace for CSCS users. There is a HiPPI network between the NEC SX-3, the Convex and between the file management software and the users' space.

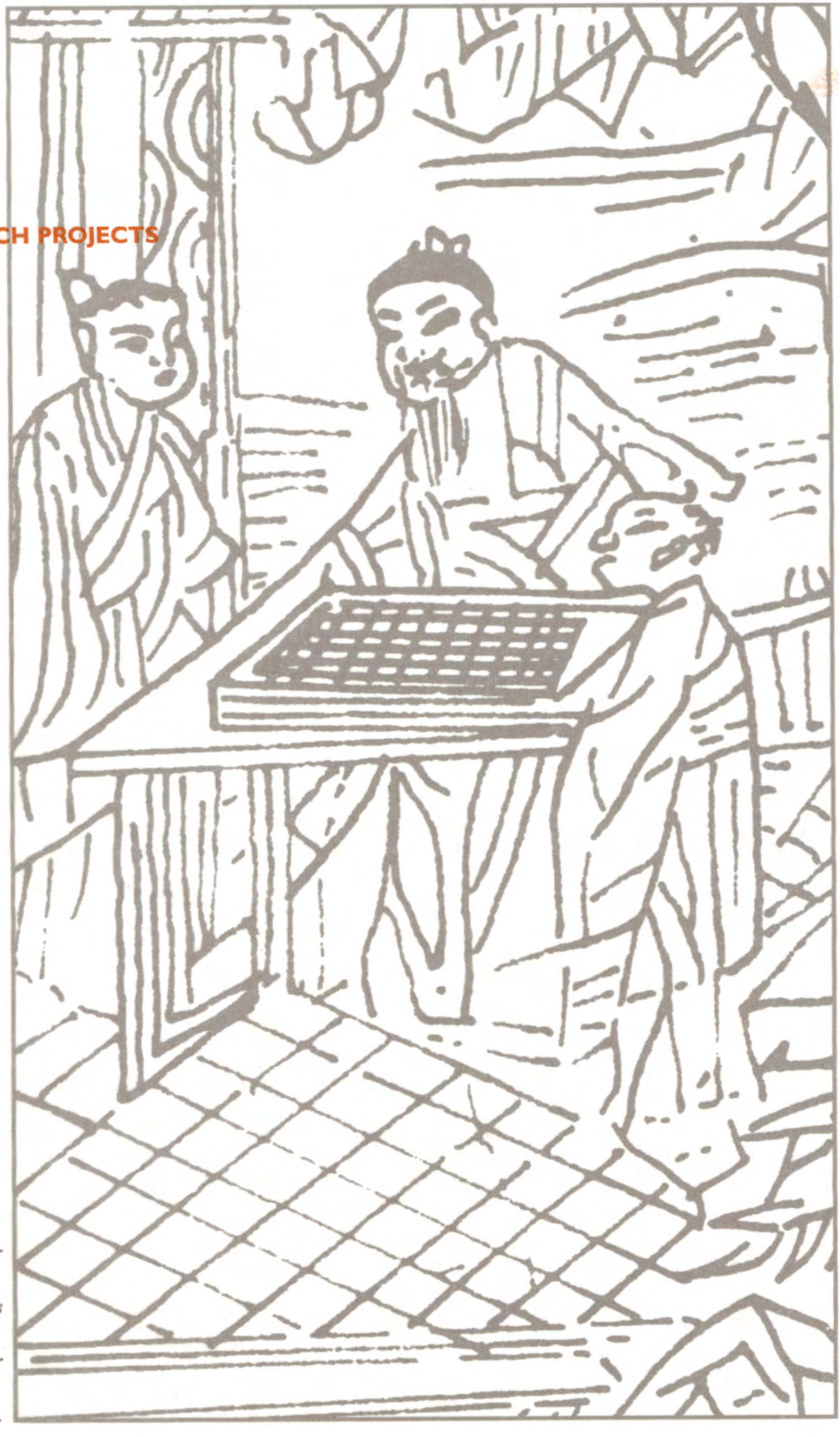
The archiving subsystem consists of two Storage Tek silos with a total capacity of 4.8 Tbytes. The upgrade to helical scan technology, planned for mid '95 will increase the available capacity by a factor of 20.

Networking

The CSCS internal network has a three FDDI ring-based architecture, implementing three hierarchical security levels. In addition, the Swiss education and research network, SWITCH, provides CSCS with an Internet connection to the world. Fault tolerant remote access to CSCS facilities is guaranteed via two 2 Mbit/s leased lines. CSCS is participating in the Swiss TELECOM PTT ATM (Asynchronous Transfer Mode) pilot project and as such is a node in the ATM network, linked to other project partners in Zurich and Lausanne (and from there to other sites) with an experimental virtual path connection (VPC). CSCS is ready to host the link for a future internal ATM network. The bandwidth for the VPC ranges from 2.5 to 20 Mbit/s.



The computer room with the vector supercomputer NEC SX-3/24R in front, the Convex 3820 in the right back and the Storage Tek archiving system on the left.



Chinese master teaching calculus on a checker abacus, 1593.

CSCS participates and conducts activities in addition to those described in the overview section. We call these activities "projects". In addition to the many projects conducted by CSCS users using the CSCS facilities, CSCS projects can include: internal projects, collaborative project efforts between CSCS personnel and other organizations, or projects conducted by visiting researchers at CSCS.

This section summarizes twenty-six CSCS projects conducted in 1994. Twenty-one project abstracts and five project reports are to be found in the following pages.

Institutes can be cross-referenced to the address list found later in this document. To assist in your reading, acronyms that appear in these abstracts and reports are fully expanded in the acronym list at the end of this document.

DYNAMIC VISUALIZATION AND SYNTHETIC IMAGE RESTITUTION FOR LARGE SCALE CIVIL ENGINEERING PROJECTS

Involved Persons:
B. Eghtessad ..... a
U. Meyer ..... b
Organizations:
a Passera & Pedretti SA
b CSCS
Funding Sources:
CSCS
Passera & Pedretti SA
Duration:
October 1994–continuing

Passera & Pedretti is visualizing part of the national Alptransit railway project in a joint collaboration with CSCS. The aim is to provide visual material and demonstrate the visual impact of the constructions (rail tracks, bridges, excavations, etc.) before they are actually built. One effective technique is to build a three-dimensional model of the rail track and merge it into a real photograph (see plate). Such highly realistic images let the observer visualize and possibly judge the effects of the rail track on the landscape.

Several specialized software packages are used to achieve this goal. The civil engineering application MOSS reads topological data obtained by different survey methods and creates a digital terrain model. Construction design and subsequent analysis are done in the same package. Initial tests gave interesting but insufficient results because the level of realism was too low. Careful evaluation of several modelling and rendering packages lead us to Wavefront's Advanced Visualizer as the most appropriate for civil engineering projects. Special attention was paid to data transfer capabilities and processing of high volumes of data. Using the Advanced Visualizer, data extracted from MOSS is combined with scanned-in real photographs to compose the final realistic image. Complete video animation sequences have been generated to further increase the realism and understanding of the project.

RACE-CONDITION DETECTION IN MULTI-COMPUTER PROGRAMS

Involved Persons:
C. Clémençon ..... a
M.J. Meehan ..... b
R. Rühl ..... a
Organizations:
a CSCS
b University of North Carolina at Chapel Hill (U.S.A.)
Funding Sources:
NEC (Germany)
Duration:
July 1994–October 1994

A type of bug unique to parallel computing can occur in message-passing parallel programs. This type of error is due to multi-message races. A race occurs when messages are in transit at the same time and the corresponding receives can accept any of the messages. Most of the time, races are intentionally incorporated into programs for reasons such as enhancing load balancing. Sometimes a race causes erroneous execution that is hard to debug because of the non-deterministic nature of the program, i.e., if the messages in a race are not received in the same order as during the erroneous execution, the error might not occur. The goal of the project is to address this problem in message-passing programs based on the MPI standard [1]. An efficient algorithm (based on [2]) for tracing a given MPI program execution and replaying that execution deterministically is designed and implemented. The tracing and replaying facilities will help the user to reexecute a nondeterministic program deterministically. This reexecutability will allow a user to gather information on and facilitate removal of all non-deterministic errors. The software developed in the project is incorporated into the PDT [3] of the *Annai* programming environment [4].

References:

[1] "MPI: A Message-Passing Interface Standard." *Message Passing Interface Forum* University of Tennessee, Knoxville, TN (May 1994).

[2] Netzer, R.H.B. and B.P. Miller. "Optimal Tracing and Replay for Debugging Message-Passing Parallel Programs." *Proceedings, Supercomputing '92* Minneapolis, MN, 502–511 (November 1992).

[3] Clémençon, C., J. Fritscher and R. Rühl. *Execution Control, Visualization and Replay of Massively Parallel Programs within Annai's Debugging Tool.* CSCS Technical Report CSCS-TR-94-09 (November 1994).

[4] Clémençon, C., A. Endo, J. Fritscher, A. Müller, R. Rühl and B.J.N. Wylie. "The Annai Environment for Portable Distributed Parallel Programming." *Proceedings, 28th Hawaii International Conference on System Sciences*, Volume II, Maui, Hawaii, U.S.A. (January 1995).

Dynamic Visualization and Synthetic Image Restitution for Large Scale Civil Engineering Projects.
Three-dimensional model of the rail track merged with a photograph.

PE²AR: PROGRAM ENVIRONMENTS FOR ENGINEERING APPLICATIONS AND RESEARCH

Involved Persons:
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G. Jost c
S. Merazzi ..... d
Organizations:
a CSCS
b SIC-EPFL
c NEC
d SMR SA
Funding Sources:
CSCS
NEC
SMR SA
Duration:
July 1994–continuing

The major goal of this project is to design and subsequently realize a software environment to ease common development of interdisciplinary programs, to integrate interdependent applications and to execute complex programs and to visualize their results. The final product will include a multiple-machine, data manager with a dynamic memory allocation system that guarantees distributed computing and a client-server concept to ease use of massively parallel computer architectures.

In a first phase, a detailed software specification is being written. This phase can profit from first experiences made with several multidisciplinary program environments such as laser optimisation, the "electrostatic precipitator" project (page 30), the fusion research environments and the integrated quantum chemistry and materials science applications.

PARALLELIZATION OF TIGHT-BINDING MOLECULAR DYNAMICS CODE

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Funding Sources:
NEC (Germany)
Duration:
July 1994–October 1994

Simulations based on the TBMD scheme [1] are characterized by significant computing time and huge memory requirements for large simulation sizes. For example, a simulation of several hundred atoms for 1000 time-steps requires more than twenty-five hours of computation time on a 64 megabytes single processor RISC workstation. To simulate 5000 atoms for 1000 time-steps within only a few hours, three tasks need to performed: reduction of the memory requirements, usage of faster numerical algorithms to calculate the required eigenvalues and eigenvectors, and parallelization for a massively parallel computer system.

To reduce the memory requirements and to improve the numerical algorithms, the sequential program was re-engineered. The sparse matrices involved in the calculation were transformed into the CSR format with the help of SPARSKIT [2]. The CSR format is also beneficial in that it allows faster calculation of eigenvalues and eigenvectors. To do the actual computation, two new subroutines from the LAPACK package were used. These two modifications result in an improved sequential TBMD program, capable of doing simulations with 1000 atoms.

The parallelization of this improved sequential TBMD program is also supported by the transformation of the data structures into CSR format, since it allows for greater data locality. The actual parallelization, using the PLUMP library [3], is currently under completion.

References:

[1] Colombo, L. "Tight-Binding Molecular Dynamics: Present Status and Perspectives." *Proceedings, Physics Computing '94* (August 1994).

[2] Saad, Y. *SPARSKIT: A Basic Tool Kit for Sparse Matrix Computation.* Technical Report CSRD 1029, CSRD, University of Illinois (August 1990).

[3] Beg, I., W. Ling, A. Müller, P. Przybyszewski, R. Rühl and W. Sawyer. "PLUMP: Parallel Library for Unstructured Mesh Problems." *Proceedings, International Workshop on Parallel Algorithms For Irregularly Structured Problems* Geneva, (August–September 1994).

PROTOTYPING A TOOL GRINDING MACHINE

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b CSCS
Funding Sources:
CSCS
Stream SA
Duration:
September 1994

The final appearance of a machine is often difficult to imagine on the basis of hand drawings and building a prototype is not always possible. Nevertheless, potential customers would like to be informed as early as possible about new machine developments and features, and often like to see a picture of the new machine.

The Advanced Visualizer software by Wavefront Technologies was used to create a prototype image of a new Stream SA tool grinding machine. A three-dimensional model was rendered by the software according to existent plans. With this model, very realistic images containing shadows and reflections are synthesized. Some parts that are too complicated to model were scanned as images from older versions of the machine (e.g., the control panel with numerous buttons and meters). The scanned images were then incorporated into the final image using the texture mapping technique.

Assignment of the "right" colors was a delicate procedure and many iterations were necessary. However, this iteration process was quite easy to accomplish once the model geometry was entered into the system.

PROGRAM STRUCTURE BROWSER FOR THE *ANNAI* INTEGRATED TOOL ENVIRONMENT

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Funding Sources:
NEC (Germany)
Duration:
July 1994–October 1994

When working with large and often unfamiliar applications, it is difficult to view the structure of a program in one glance. Studying the code within one subroutine itself becomes difficult because of the size of the code. Analysis becomes even more difficult once there is additional information associated with a code block, such as performance statistics. In such cases, it is useful to have a browser which can display the program in a concise form.

The program structure browser is designed for this purpose. It provides features to navigate through the program, hide code blocks that the user is not currently interested in, and mask program statements of a specified type (such as straight-line code or calls to intrinsic routines). The structure browser is an integral part of the *Annai* programming environment. It interacts with other tool components like the PMA to display performance statistics such as execution counts, execution times, and communication overheads as tabular annotations. The browser provides facilities to sort routines based on these statistics. Tools of similar nature are provided in Thinking Machines' Prism and Cray Research's MPP Apprentice.

References:

[1] Clémençon, C., A. Endo, J. Fritscher, A. Müller, R. Rühl and B.J.N. Wylie. "The Annai Environment for Portable Distributed Parallel Programming.", *Proceedings, 28th Hawaii International Conference on System Sciences–volume II* edited by H. El-Rewini and B.D. Shriver. Computer Society Press (1995).

[2] Sistare, S., D. Allen, R. Bowker, K. Jourdenais, J. Simons and R. Title. "Data Visualization and Performance Analysis in the Prism Programming Environment." *Programming Environments for Parallel Computing* edited by N. Tophan, R. Ibbett and T. Bemmerl. 1992: pp. 37–52.

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Prototyping a Tool Grinding Machine. Prototype design of a heavy metal tool grinding machine.

GLOBAL DATA VISUALIZATION FOR DEBUGGING DATA PARALLEL PROGRAMS

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Funding Sources:
NEC (Germany)
Duration:
July 1994–October 1994

Data-parallel languages such as HPF allow programmers to specify how data structures are aligned relative to each other and then distributed across many processors. Program performance is often directly related to how data have been distributed, and a means of evaluating data distribution and alignments is essential. The software developed in this project provides three displays to visualize distributed data: the first one displays a colored cell for each array element, where each processing element is denoted by a different color; the second one shows in addition the value of the array element in each colored cell, and the third one provides a three-dimensional representation of the array, where the first two dimensions depict the grid of processor elements and the value of the array element is presented in the third dimension.

References:

[1] Allen, D., R. Bowker, K. Jourdenais, J. Simons, S. Sistare and R. Title. "The Prism Programming Environment." *Proceedings, Supercomputer Debugging Workshop '91* Albuquerque (November 1991).

PARALLEL PROGRAMS WITH THE TINA-2 FRAME LANGUAGE

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NEC (Germany)
Universität Basel
Duration:
July 1994–October 1994

During the past years, the Computer Science Department of the University of Basel has developed a classification scheme for parallel algorithms, called BACS. On one hand, BACS allows the teaching of parallel algorithms by reducing them to important structures. On the other hand, it allows searching and retrieving algorithms from BALI for programming purposes. BALI collects and describes algorithms which not only use BACS but also natural language and a programming language called ALWAN. The ALWAN language (former *FRAME*) itself is based on BACS and supports structured programming as well as portability of codes at low costs. The first part of this project covered the introduction to these three topics.

In the second part, some smaller algorithms were studied, described and put into BALI. They primarily included algorithms from mathematics and physics, such as a root search or a radiosity simulation. Finally, two application-oriented problems were treated: the first dealt with "generalized quadrangles" using a pipe topology, the second with "kinetic gas simulation" using a cubic torus.

It has to be said that, at the time of this work, no complete ALWAN compiler was available.

This project was carried out within the framework of SSIP'94.

References:

[1] Burkhart, H., C.F. Korn, S. Gutzwiler, P. Ohnacker and S. Waser. *BACS: Basel Algorithm Classification Scheme.* Technical Report, Computer Science Department, University of Basel, October 1992.

[2] Burkhart, H., W. Kuhn and P. Ohnacker. *BALI, The Basel Algorithm Library* Technical Report, Computer Science Department, University of Basel (in progress).

[3] Burkhart, H., R. Frank, G. Hächler, P. Ohnacker and G. Prétôt. *ALWAN, Programmer's Manual* Technical Report, Computer Science Department, University of Basel (in progress).

[4] Hächler, G. and H. Burkhart. "Programmability, Portability and Performance of Parallel Systems: The Basel Approach." SPEEDUP Journal 8(2) (December 1994): 31–38 .

[5] Dold, A. "Parallelisierung eines Programmes aus der diskreten Mathematik." University of Karlsruhe (1994).

3D MHD EQUILIBRIUM CODE CLIO 3D

Involved Persons:

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Funding Sources:

CRPP-EPFL
CSCS
MPI für Plasmaphysik
Keldysh Institute of Applied Mathematics

Duration:

January 1994–December 1995

CLIO 3D is an ideal magnetohydrodynamic equilibrium program to compute the input quantities needed for the 3D MHD stability code TERPSICHORE. The major goal is to compute new stable thermonuclear fusion configurations with the most advanced confinement properties.

The existence of ideal 3D MHD equilibria has not yet been mathematically demonstrated. Adding non-ideal physical effects (such as ion Larmor radius effects) to the ideal model brings the model back to a physically relevant one. Until now, the major effort was to find the physically and mathematically correct formulation of the equations that would allow a converging numerical approach. A first prototype of CLIO 3D has been applied successively to compute the analytic 2D Solovev equilibrium solution.

CRYSTALLIZATION IN A FLOW

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Funding Sources:

CSCS
ETHZ

Duration:

July 1993–December 1995

The goal of this project is the numerical simulation of crystallization in various flows with regard to a space-dependent CSD. A model for such a process must take into account the reciprocal effects of the following subprocesses: mixing due to convection and diffusion, chemical reaction, and crystallization (which consists of nucleation and crystal growth).

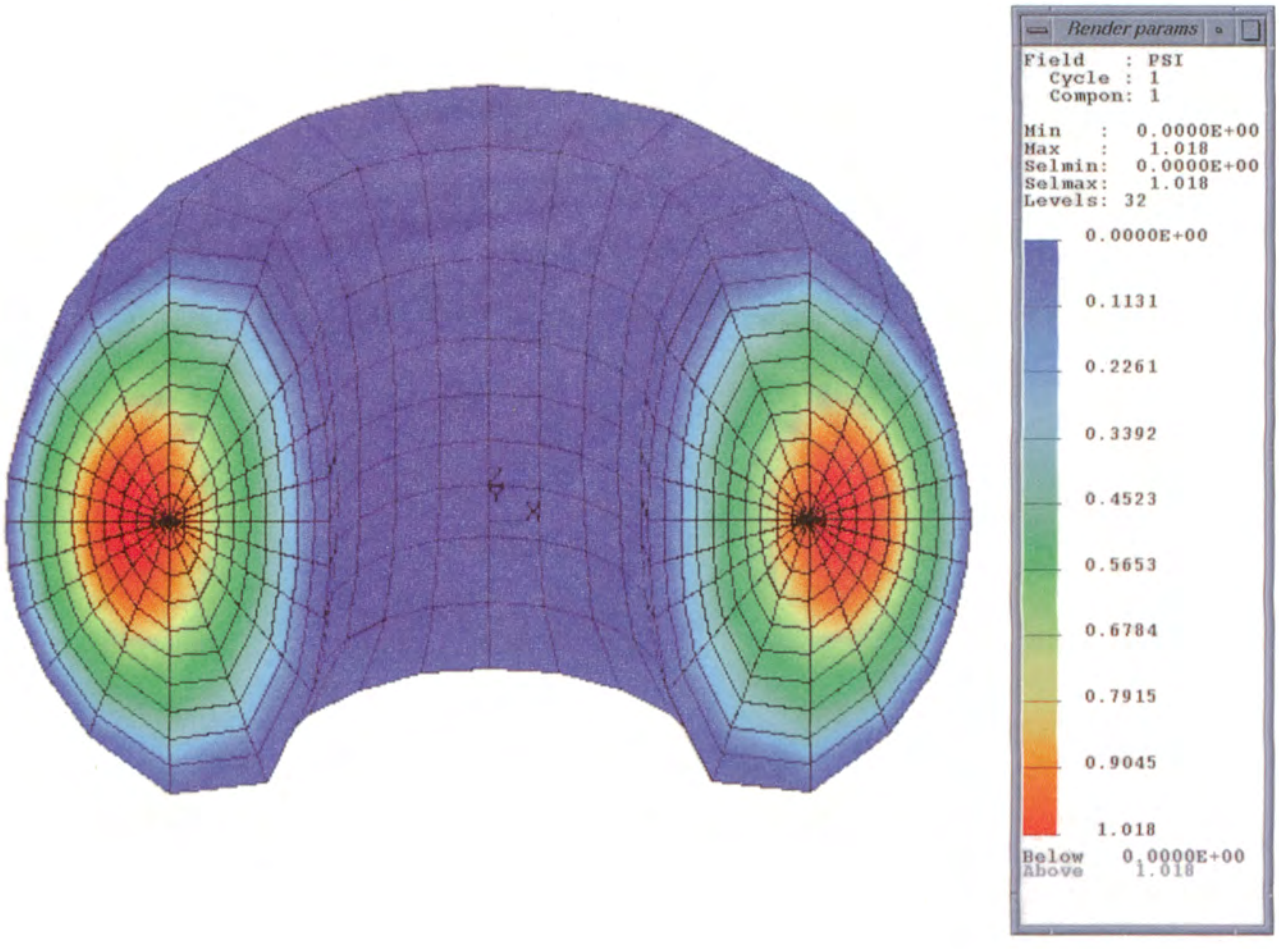
Different mixing behavior is simulated by different reactor types. The stirred tank reactor represents the limiting case of ideal mixing whereas in a plug flow reactor convective mixing occurs. More detailed studies are possible for a continuous reactor with two separated entrance flows.

For the chemical process the single second order reaction (A+B->P) between two species which form a poorly soluble product has been chosen. No by-products are formed.

The crystallization of a substance from a supersaturated solution is influenced not only by the parameters of the solution but also by the crystals themselves. The model considers secondary nucleation and the dependency of the crystal growth rate on the supersaturation. Other influences are averaged in the rate constants.

The mass balances for the solved substances and for the CSD are solved with a maximum of two spatial coordinates and one internal coordinate (crystal size) using the QUICKEST algorithm in combination with the ULTIMATE limiter. This method has a low numerical dissipation and therefore it is suitable for the simulation of fields with large gradients. Since their steepness is limited by the grid resolution, moving concentration fronts still cannot be represented accurately enough with fixed grids in large computational domains.

In that case the application of an adaptive grid method has shown good results. It is developed for steady state calculations for one spatial and one internal coordinate and is extended with some restrictions to a second spatial coordinate.



3D MHD Equilibrium Code CLIO 3D.

COUPLED MOTION OF ELECTRONS AND ATOMS ON THE SI(001) SURFACE

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Funding Sources:
Universität Basel
Universität Zürich
Duration:
March 1994–December 1995

In this project the *ab initio* molecular dynamics in the Car-Parrinello formulation has been applied to study the microscopic processes in semiconducting materials and the scientific visualization tools have been developed in order to animate the emerging dynamical picture. These tools can now be offered to all CSCS users performing the MD simulations for solid state physics and materials science.

The coupled evolution of the atomic positions and of the electronic density of the highest occupied states on the Si(001) surface have been studied by first-principles molecular dynamics [1]. A video sequence illustrating the time-dependent changes accompanying the anharmonic flipping of dimers in the top layer has been generated using the SGI Explorer graphics package. The experimental facts that at room temperature the dimers appear symmetric in scanning tunnelling microscope topographic images [2], whereas at low temperatures (T<120K) dimers appear tilted [2, 3] are confirmed [4, 5, 6] (see Figure).

Moreover, the incomplete shielding of the lower atoms of tilting dimers induces an electronic polarization and compensating lateral displacements of adjacent Si atoms in the second layer. A coupling of the corresponding surface vibrations should be observable. Similar molecular dynamics calculations will be extended to defects and to alkali-metal adsorbed on the same silicon surface.

References:

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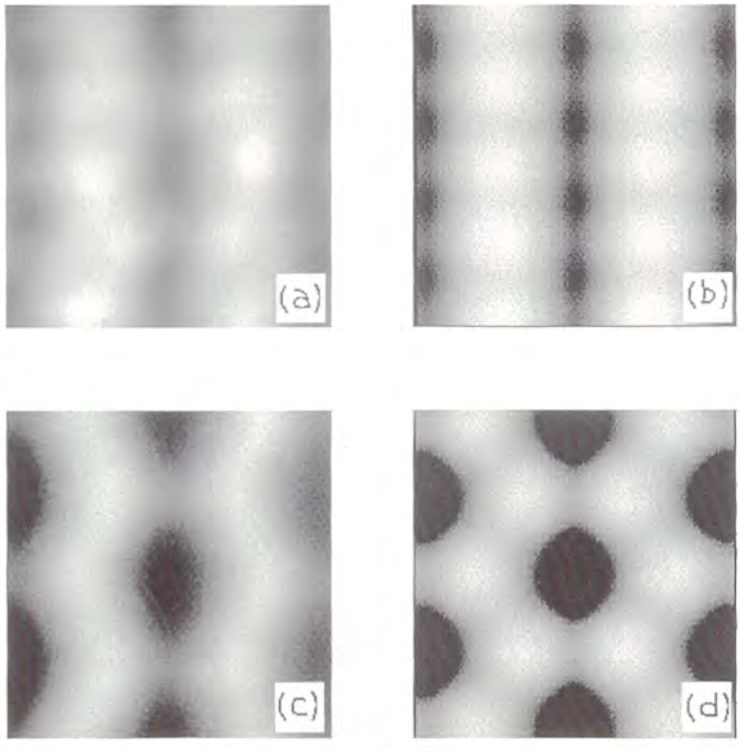
[3] Meyer, G. and K.H. Rieder. *Private communication.*
[4] Stoll, E.P., A. Baratoff, A. Mangili and D. Maric. *Proceedings, 6th joint EPS-APS International Conference on Physics Computing* edited by R. Gruber and M. Tomassini. European Physical Society, Petit-Lancy, 1994, p. 33.
[5] Stoll, E.P., A. Baratoff, A. Mangili and D. Maric. Lecture Notes of the 18th Gwatt Workshop *Computational Physics and Chemistry* Sept. 29–Oct. 1, 1994, Gwatt, Switzerland.
[6] Stoll, E.P., A. Baratoff, A. Mangili and D. Maric. *Helv. Phys. Acta* (to be published).



Gray-scale images of adjacent dimer rows on Si(001); (a) and (c): STM topographs recorded at room temperature [2] and at 64 K [3]; (b) and (d): computed images at about 220 K and at about 70 K.

COMPUTER-GENERATED EDUCATIONAL VIDEO SEQUENCES

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R. De Gaetano ..... b
S. Giordano ..... a
M. Magni ..... b
A. Mangili ..... a
G. Monza ..... b, c
R. Peterhans ..... b
I. Pontiggia ..... a
A. Rordorf ..... b
F. Russo ..... b
K. Walder ..... b, c
I. Wolf ..... b

Organizations:

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b CSIA
c DIC, Divisione della formazione professionale del canton Ticino

Funding Sources:

CSCS
CSIA
DIC

Duration:

July 1994–March 1995

CSCS is collaborating with CSIA to realize several computer-generated sequences for educational purposes. Subjects and contents cover a wide topic area in the field of computer science (e.g., mathematical models and simulation, supercomputers, parallel computers, network, and visualization).

The CSIA students are realising these computer-generated sequences as a semester project. The main goal of the project is to produce a professional video clip—from concept to the practical implementation. The realization is accomplished using specific software tools for three-dimensional objects modelling and image synthesis.

These sequences will be used by CSCS for its educational program during site visits to explain the major activities and problems related to computer science in a simple and visual way .

Reference:

Moor-Häberling, C., R.M. Rehmann and B.J.N. Wylie. "Project Proposal: CSCS Education Program: School Visits." CSCS-ETHZ (1994).

PARALLELIZATION OF SOLIDIS

Involved Persons:

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c CSCS

Funding Sources:

NEC (Germany)

Duration:

July 1994–October 1994

SOLIDIS is a package of finite element computational kernels and front-end visualization programs used to solve, for instance, the charge transport equations in semiconductors relevant for integrated microsystems. SOLIDIS is based on the SESES system, which is elucidated in two ETH dissertations [1, 2].

The time consuming parts of the program are the construction and the solution of the linear system. The goal of this project was to conquer both problems by parallelization. The linear systems can be solved using the iterative KSM solvers (from the SPARSKIT package) and the corresponding parallel kernels (PKK) developed in another project at CSCS (see "Parallel Kernels for Krylov Subspace Methods" page 29). The parallel KSM solvers allow an efficient parallel matrix assembly which traverses two steps: the construction of the indices for non-zero entries of the matrix (index assembly) and the collection of the matrix coefficients (stiffness assembly). This is suitable for the compressed sparse row (CSR) or other distributed matrix format.

The code is written in C with MPI calls, except for the linear solvers which are implemented in FORTRAN. The graphical front-ends require the X-windows library in addition to the standard C libraries. The parallel version was developed on the 4 processor SPARC server and ported to the NEC Cenju-3.

References:

[1] Korvink, J. "An Implementation of the Adaptive Finite Element Method for Semiconductor Sensor Simulation." Ph.D. thesis, ETH-Zürich, November 1993, Verlag der Fachvereine Zürich, Report Nr. 8.

[2] Sartoris, G.E. "A Hybrid Finite Element Method to Solve the Stationary Semiconductor Equations Including Galvanometric Effects." Ph.D. thesis, ETH-Zürich, November 1993, Verlag der Fachvereine Zürich, Report Nr. 7.

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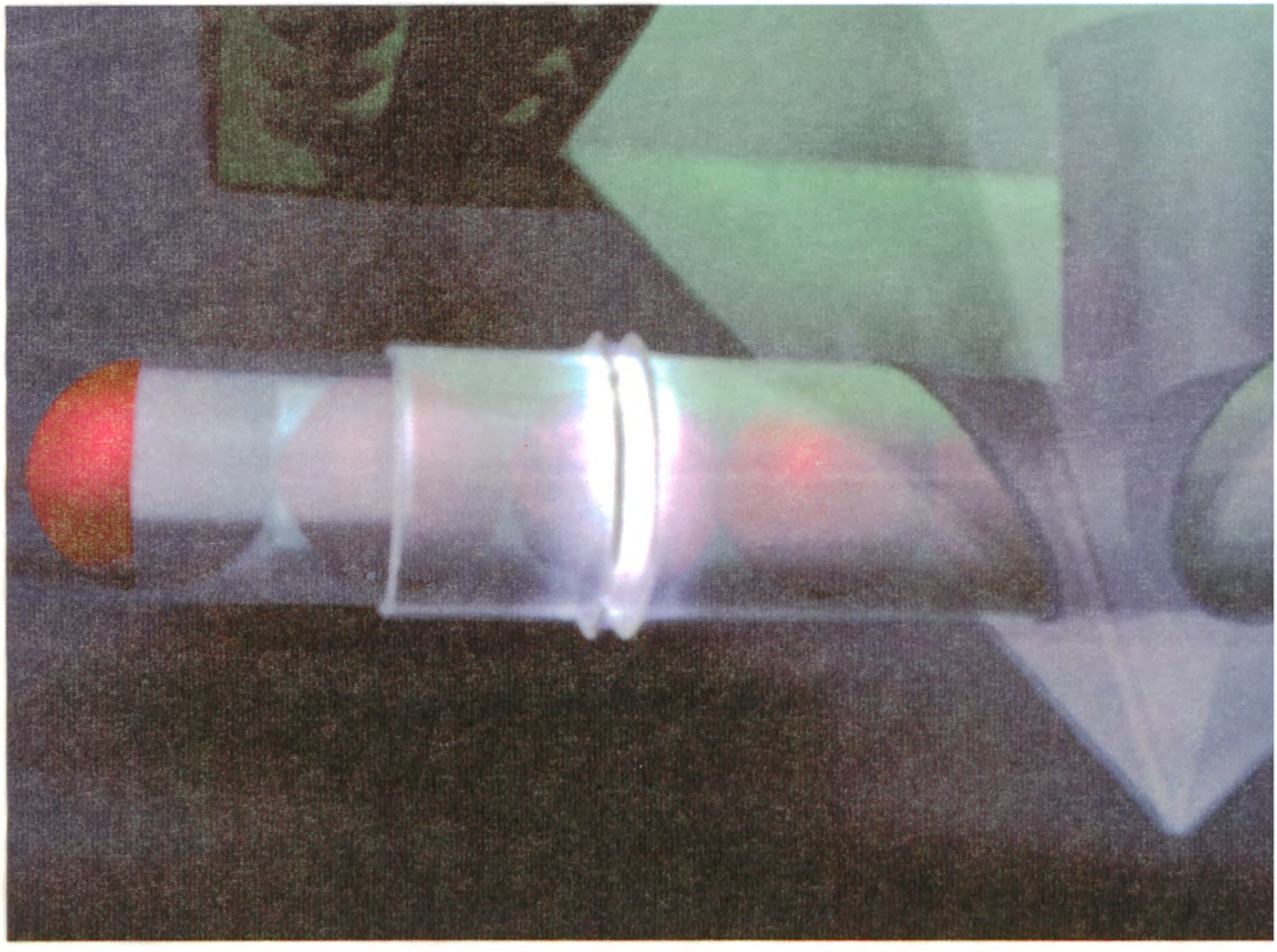

Computer-Generated Educational Video Sequences. Image taken from a video sequence showing the capability of errors detection during packet data transmission. The network is represented by tubes, packets of data are represented by balls.

TELE-WORKING AND TELE-CONFERENCING TOOLS FOR USER SUPPORT

Involved Persons:
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S. Klett ..... a
A. Mangili ..... a
Organizations:
a CSCS
Funding Sources:
CSCS
Duration:
October 1994–continuing

Technologies such as video-conferencing and tele-working allow people to communicate and cooperate in a project while significantly reducing the costs. Video-conferencing allows participation in a meeting or a conference without travelling; tele-working offers real-time, shared access of the same document to a group of people physically located in different sites.

CSCS is following these technology innovations for improving user support. A first trial was conducted in November 1994 at the TELECOM PTT public videoconferencing room in Manno. An ISDN link was setup to allow participation in a video-conference organized during the Al Tecnologie exhibition, a conference on new technologies for the productive process held in Italy. The test was satisfactory and it proved that a low cost ISDN line could be used for video-conferences.

A second follow-up test was made in December 1994 during the evaluation of a tele-working tool. A dedicated ATM connection was setup between EPFL and CSCS, making it possible to give a seminar remotely via Internet to a wide audience. We were also able to prove the feasibility of remote user support and collaboration in a user project using tele-conferencing and tele-working tools. The major advantages are: real-time interaction from users' desktop, real-time sharing of documents and applications between users, and multi-point connection of physically diverse sites. Currently this technology suffers from several limitations: network speed, software and hardware incompatibility (due to heterogeneous platforms using different standards), multimedia devices that are not always available, and lack of true interactive distributed applications.

This project will be continued to evaluate the improvements of using ATM connections, the limits of ISDN (2B+D), and the benefits of interactive distributed applications and tele-education.

References:

[1] In *Person User Guide* Silicon Graphics Inc. (1994).
[2] In *Person Setup and Administration Guide* Silicon Graphics Inc. (1994).

PARALLEL FRACTAL IMAGE COMPRESSION USING ITERATED FUNCTION SYSTEMS

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NEC (Germany)
Duration:
July 1994–October 1994

Compressing an image by fractals consists of finding self similar parts in the image and storing only the transformation between these parts. This technique has the advantage of obtaining high compression ratios. Its disadvantage is that the encoding step is computationally expensive. A large number of sequential searches through a list of image parts are carried out while trying to find a best match for a portion of the image. To reduce this enormous computing time a parallel algorithm for fractal image compressing is presented, implemented on a NEC Cenju-3 using MPI for message passing.

The idea of representing images as transformations that generate them was first proposed by M. Barnsley [1]. Many natural objects such as trees, clouds, mountains or leaves can be approximated by fractals. Barnsley proposed the use of the theory of iterated function systems (IFS) to create fractal shapes.

The transformations in all IFS are contractive transformations on the space of images. The transformation applied to an image produces a new image. If the transformation is contractive then recursive application of it onto an arbitrary image produces the fixed point of the transformation. The basic problem in fractal coding methods is to calculate a transformation for a given image. Since the encoding algorithm is typically computation-intensive, the idea is to reduce the

encoding time by parallelization. The code used in this project is originally from Carnelli [2]; this work was conducted in collaboration with the Human Capital & Mobility Program (see page 38).

References:

[1] Sloan, A. and M. Barnsley. "A Better Way to Compress Images." *BYTE* (1988).
[2] Carnelli, L. "Compressione Frattale di Immagini." Università degli studi di Milano, 1992/1993.
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COMPUTER-AIDED DRUG DESIGN: QUANTITATIVE STRUCTURE-ACTIVITY STUDIES OF ANTIMALARIAL COMPOUNDS RELATED TO ARTEMISININ

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H.U. Suter ..... b
C. Thomson c
J. Weber ..... d
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d Département de Chimie Physique, Université de Genève
Funding Sources:
Helmut Horten Stiftung
Duration:
May 1994–November 1995

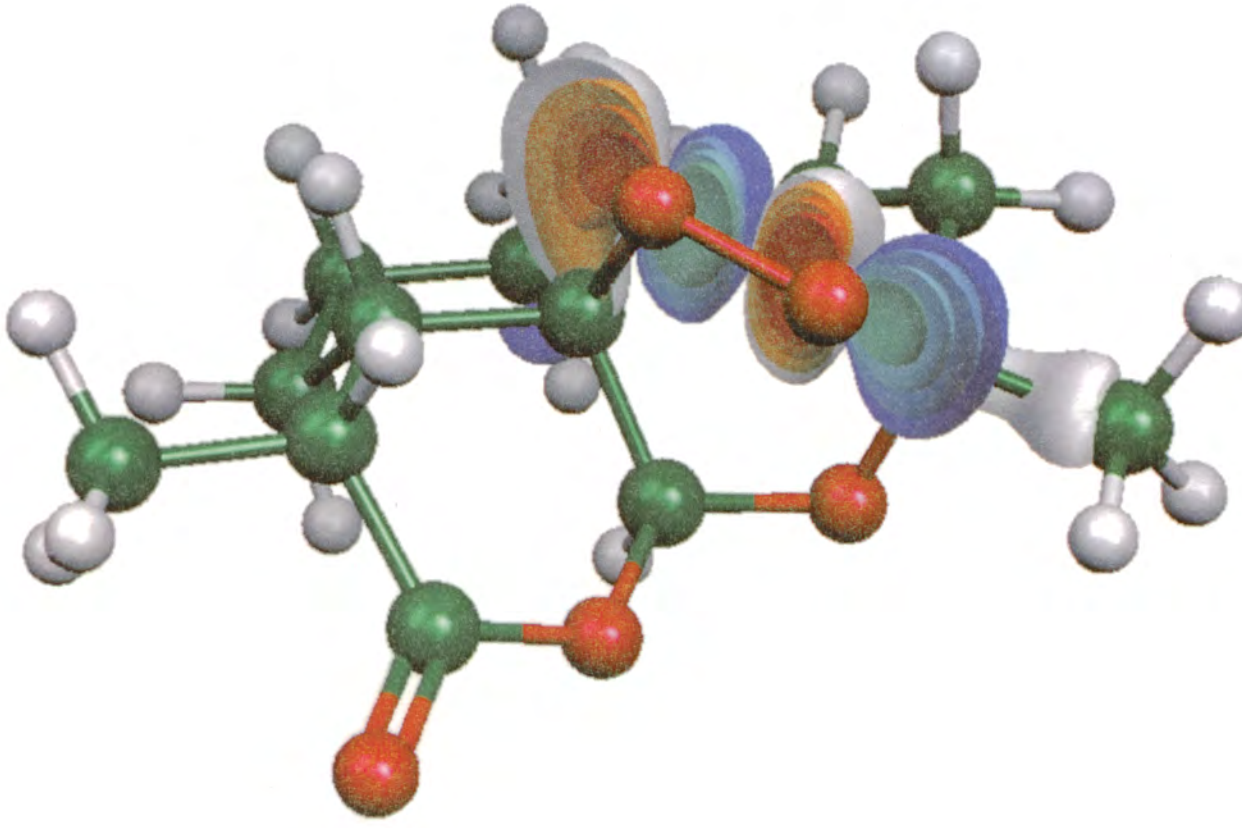
The average development time of a new drug is twelve years, at a cost which may reach 150 million dollars [1]. It is therefore of utmost importance to investigate new directions in drug design which might reduce both development time and cost. Although no single drug has yet been designed solely using computer techniques, the contribution of these methods to drug discovery is no longer matter of dispute [2]. The purpose of our project is to investigate the capabilities of current state-of-the-art quantum chemistry methods, as implemented on the CSCS high-performance computing infrastructure, in this promising field.

The discovery that artemisinin, a naturally occurring 1,2,4-trioxane extracted from the Chinese herb qinghaosu, exhibits potent antimalarial properties has provided a potential lead for the development of improved analogues [3]. Considerable efforts have thus been spent recently in the search of novel systems related to artemisinin with higher antimalarial activity.

A good example is found in the Department of Organic Chemistry at the University of Geneva, where the group of Prof. C.W. Jefford has synthesized and characterized a vast series of compounds (structurally) resembling artemisinin in an attempt to design better drugs. The availability of their data has prompted us to perform theoretical studies in an attempt to find possible correlations between the structure and the activity of the most prominent members of this family of compounds [4]. To this end, *ab initio* quantum chemical calculations have been performed on the NEC SX-3. After a geometric optimization of the these compounds (i.e., a determination of their most stable conformation), additional calculations of the detailed features of their electrostatic potentials on molecular surfaces were carried out [5]. Kohonen maps derived from neural networks were then used to compare the two-dimensional characteristics of these potentials and to define possible correlations between the structure of the systems and their activity. Such investigations should help to provide insight into the mechanism of action of artemisinin and, ultimately, to propose new synthetic targets.

References:

[1] Carey, J. "New Resolutions in Drug Design." *Chem. Britain* 29(1993): 1053.
[2] Richards, W.G. "Computer-Aided Drug Design." *Pure & Appl. Chem.* 66(1994): 1589.
[3] Butler, A.R. and Y. Wu. "Artemisinin (Qinghaosu): A New Type of Antimalarial Drug." *Chem. Soc. Reviews* (1992): 85.
[4] Suter, H.U., D.M. Maric, J. Weber and C. Thomson. "Quantum Chemistry and Drug Design." Crosscuts 3 (1994).
[5] Bernardinelli, G., C.W. Jefford, D. Maric, C. Thomson and J. Weber. "Computational Studies of the Structures and Properties of Potential Antimalarial Compounds Based on the 1,2,4-Trioxane Ring Structure. I. Artemisinin-like Molecules." *Int. J. Quantum Chem. Biol. Symp.* 21 (1994): 117.



Computer-Aided Drug Design. Quantitative structure-activity studies of antimalarial compounds related to artemisinin have shown that the unoccupied orbital of the O-O bond attracts an electron and so becomes responsible for the activity of these drugs.

PROGRAMMING ENVIRONMENT FOR PARALLEL ITERATIVE SOLVERS

Involved Persons:
J.J. Dvorak ..... a
R.M. Rehmann ..... a
T.S. Toupin ..... b
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NEC (Germany)
Duration:
July 1994–October 1994

Iterative solvers which attempt to find approximate solutions to the matrix equation $y = Ax$ (for sparse matrices arising from typical scientific applications) can be described by sequential programs which make use of a set of kernel matrix operations [1]. Though the functionality of these kernel matrix operations is easily described, each operation must have multiple implementations due to the various existing data structures for sparse matrix storage.

Parallelizing these iterative solvers generally, the focus of the parallelism must be with the kernel matrix operations [2] since the process of the iterative solvers is inherently sequential and lacking any generalizable parallelization. Yet the process of parallelization of the kernel matrix operations becomes immediately difficult since parallel kernel matrix operations now have multiple implementations due not only to the data structures for the sparse matrix storage, but also to the desired parallel data distribution scheme. The solution which emerges from this problem is a parallel programming environment [3] that allows users to develop iterative solvers in an abstract way using a specification language called BLIPS which the user can modify and extend. The programming environment then selects the kernel matrix operations which are most suited to the initial abstract problem specification, the structure of the sparse matrices and the desired data structures, and produces an executable C program.

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GRAPHICAL USER INTERFACE ON TOP OF THE FTP SERVICE FOR THE PECCAM CHEMISTRY PROJECT

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Duration:
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The project *Optimal User Support by PECCAM* [1] is a large application developed for the remote execution of computational chemistry packages on a network of heterogeneous computers, and for the visualization of molecular structures and properties.

For security reasons imposed by some computing centers the access is strictly limited to TELNET and FTP. Having a simple and intuitive graphical user interface for browsing in the directory structure and transferring files became fundamental in the context of the PECCAM project.

The aim of this phase was to design and develop a user interface for the FTP service, using XF an interactive graphical user interface builder working on new emerging interface technologies (Tcl/Tk).

Milestones achieved:

- conception and design of the user interface,
- implementation of design concept using the interactive graphical user interface builder,
- critical evaluation (weakness/strengths of the choices made), and
- testing.

The result is a user-friendly, file browser-like interface integrated in the PECCAM project for the transfer of inputs and outputs files between the different computers.

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PRDDO/M ON THE NEC SX-3: APPLYING NON-EMPIRICAL QUANTUM MECHANICS TO EXTREMELY LARGE MOLECULES

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Duration:

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In *Crosscuts* [1] we reported our progress in optimizing PRDDO/M on the NEC SX-3. PRDDO/M is an approximate *ab initio* code which closely reproduces the results of *ab initio* calculations with a minimum basis set of Slater orbitals in a fraction of the computational time. Because PRDDO/M is highly vectorizable, we were able to develop a SX-3 version of the code which is extremely efficient. This has allowed us to routinely apply non-empirical quantum mechanics to molecular systems that are far larger than the best *ab initio* codes can handle.

For very large systems, PRDDO/M runs at a sustained rate of about 1 GFLOPS on one CPU of the SX-3, and is 50–100 times faster than a STO-3G calculation, with near-quantitative agreement in the calculated molecular properties. A typical example of this performance is a PRDDO/M calculation on the hydrogen-saturated diamond cluster $C_{504}H_{210}$ (2730 basis functions), which requires about six hours of CPU time and runs at over 950 MFLOPS. Another example is the thirteen base pair DNA fragment (see Plate) with a molecular formula of $C_{253}H_{347}O_{152}N_{98}P_{24}$ and 3051 basis functions, which requires 6.2 hrs of CPU time. Perhaps even more significant, the combination of PRDDO/M and the SX-3 allows calculations in the range of 1000 basis functions to be done very rapidly. For instance, a 19 amino acid sequence taken from the G alpha helix of sperm whale myoglobin containing 330 atoms and 973 basis functions runs in only 15 minutes.

Further developments in the PRDDO/M methodology, particularly the implementation of pseudopotentials, will increase the performance of the method beyond what is reported here. Applications of the method extend to many chemical, biochemical, and materials science problems.

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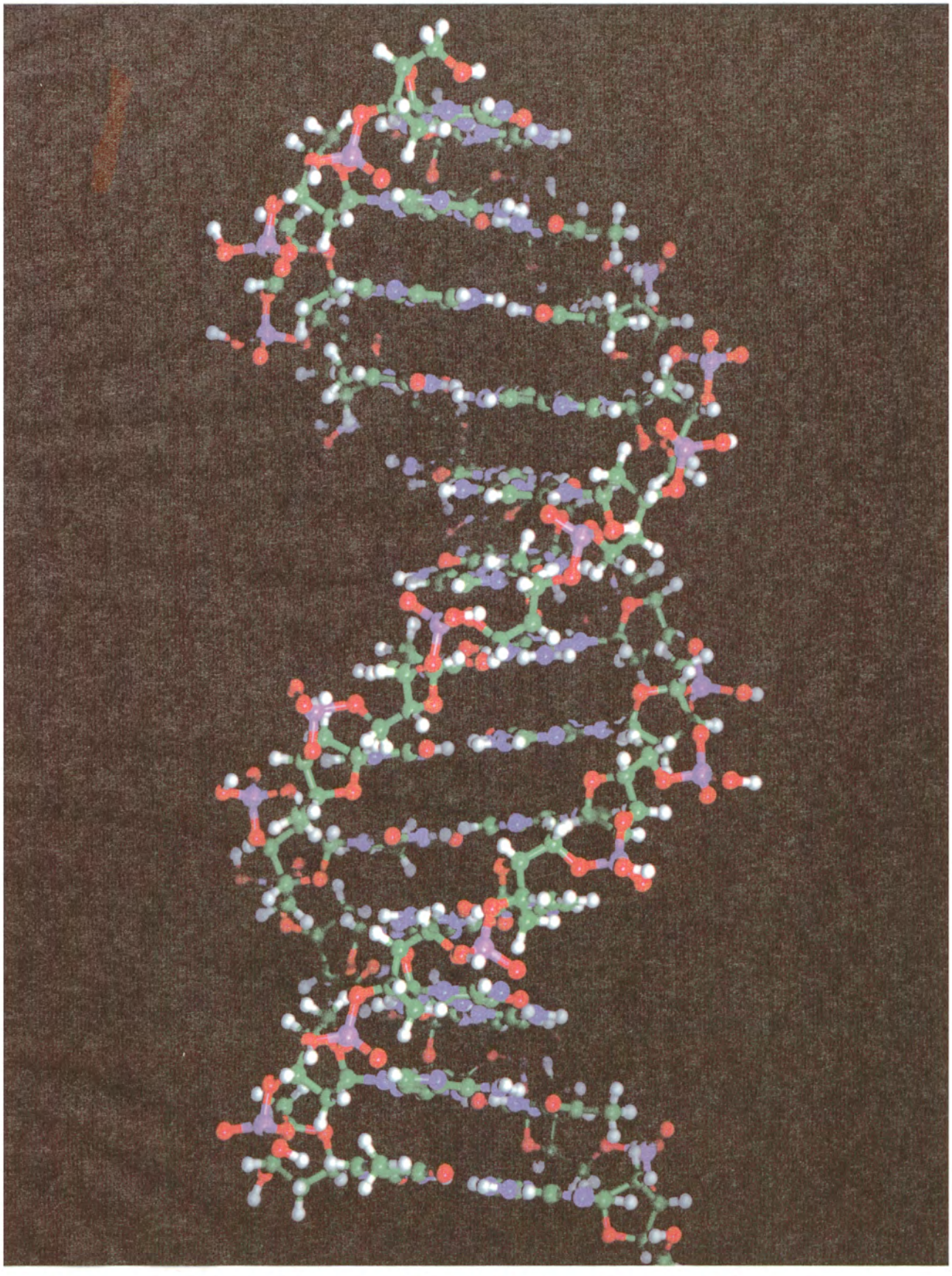
[1] Marynick, D.S., A. Derecskei-Kovacs, S.K. Estreicher, M.A. Roberson and D. Maric. *Crosscuts* 3 (1) (1994).



PRDDO/M on the NEC SX-3: Applying Non-Empirical Quantum Mechanics to Extremely Large Molecules. Thirteen DNA base-pair sequence gaatggggacgat. The compliment strand, phosphates and sugars are included (3051 orbitals).

PLUMP–PARALLEL LIBRARY FOR UNSTRUCTURED MESH PROBLEMS: TECHNICAL SPECIFICATION

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NEC (Germany)
Duration:
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The Joint CSCS-ETH/NEC Collaboration in Parallel Processing is creating a tool environment for porting large and complex codes to massively parallel computers. Along with a parallel debugger and a performance monitor, this environment provides a parallelization support tool (PST) to supplement the data-parallel programming language HPF. Whereas HPF has only facilities for regular data decompositions, PST supports user-defined mappings of the global name space to individual processors, allowing for the parallelization of unstructured problems.

Since the additional directives of PST alone do not remove all of the complexity of programming parallel unstructured mesh applications [1], a parallel library for unstructured mesh problems (PLUMP) is currently being developed at CSCS to support the local refinement and dynamic repartitioning of meshes distributed over a processor array. The constituent routines simplify the manipulation of the underlying dynamic data structures. The use of PLUMP in conjunction with PST can facilitate the design and implementation of a class of specific, but industrially important, applications.

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PARALLEL KERNELS FOR KRYLOV SUBSPACE METHODS

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This project involved the design and implementation of a set of generic basis routines and data structures implement KSM. The routines and data structures are generic in the sense that they support different matrix storage formats, different iterative methods, and different preconditioners (also in different storage formats). In addition, different distributions (within certain limits) are supported as well. The parallelism is handled within the subroutines so that a user may provide either a global matrix and a distribution scheme, or generate the distributed parts of the global matrix in place and provide the chosen distribution. The subroutines will take care of all initialization and organization of the parallel implementation. Not all options have been implemented, but extension is straightforward [1, 2]. These kernels facilitate the quick, efficient, and portable implementation of a variety of parallel Krylov subspace methods. The kernels have been used for the implementation of the parallel KSM package, which is based on both the kernels and the Sparskit2 package [3]. The kernels and the KSM package are described in detail in [1] and [2].

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COMPUTATIONAL MODEL FOR AN ELECTROSTATIC PRECIPITATOR

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ABB

Duration:

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1. Introduction

An electrostatic precipitator (ESP) is a facility used in power and waste incineration plants to eliminate fly ash particles from the flue gas (Plate 1). An ESP consists of several rectangular channels with high-voltage discharge electrodes of various shapes mounted in the middle plane parallel to the channel walls and perpendicular to the flow direction. Polluting particles in a gas that flows through these channels can be precipitated by charging them with ions from the corona region of the electrode. In the electric field the charged particles migrate to the grounded channel walls where they are deposited and finally removed.

Some of the important physical properties are the electric field, the space charge, the flow velocity field, the particle charge and particle size which all are nonlinearly interlinked by corresponding physical laws. CSCS, collaborating with ABB Corporate Research, is establishing a computational model to enable the simulation of an ESP targeting to improve the efficiency of future installations. The numerical simulation of the ESP-behavior is challenging because of the above described multi-disciplinary nature of the problem, where knowledge of specialists in different fields of physical modeling has to be combined. A data base concept, so-called PE²AR [1] (Figure 1) is used for enabling an efficient interaction of programs which have been developed independently by the various researchers.

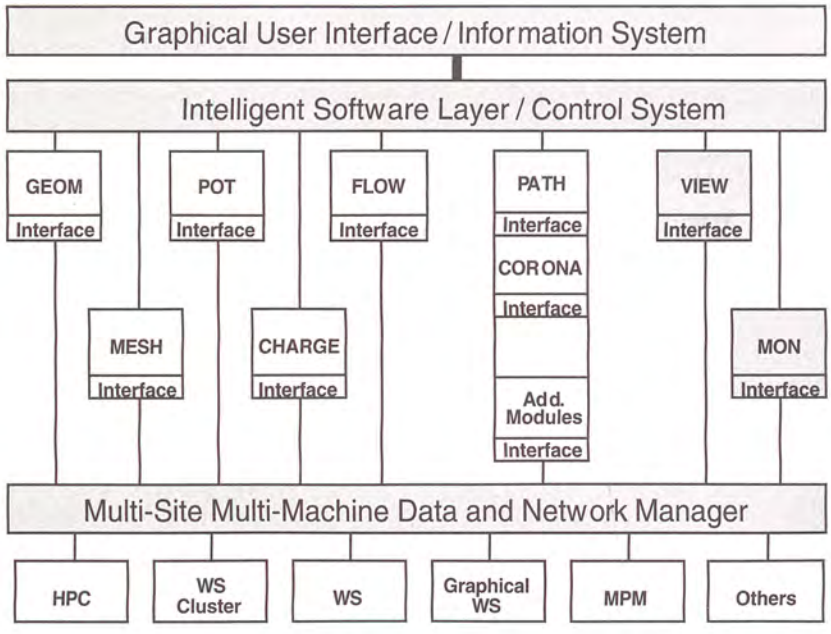

Figure 1. PE²AR programming environment for a computational model of an ESP.

The geometry definition (GEOM), the mesh generation (MESH) and the solution of the electrical potential (POT) are carried out by using the ASTRID [2] system, which can be seen as a conceptional predecessor of the above mentioned PE²AR environment. More recently, a method for calculating the self-consistent charge density distribution [3] and flow simulation modules have been implemented into the environment. One example for the multi-disciplinary interaction of modules is the consideration of additional source terms for momentum and energy in the fluid equations, which are electrical forces (space charge multiplied by the electrical field vector) and mechanical drag forces of particles. The mechanical forces result from the motion of the charged particles relative to the gas (Stokes forces). Accordingly, the flow module has to interact with the modules calculating the electrical behavior as well as with the module which simulate the particle path.

2. Computational Mesh and Data Structure

For the generation of the computational mesh, an ASTRID module (MESH) is applied based on the usage of arbitrarily connected structured mesh blocks. This approach combines the geometric flexibility of an unstructured approach with the computational efficiency of a structured discretization scheme. However, special care has to be taken by implementing block-structured methods, in order to ensure a proper continuation of the space operators across internal block

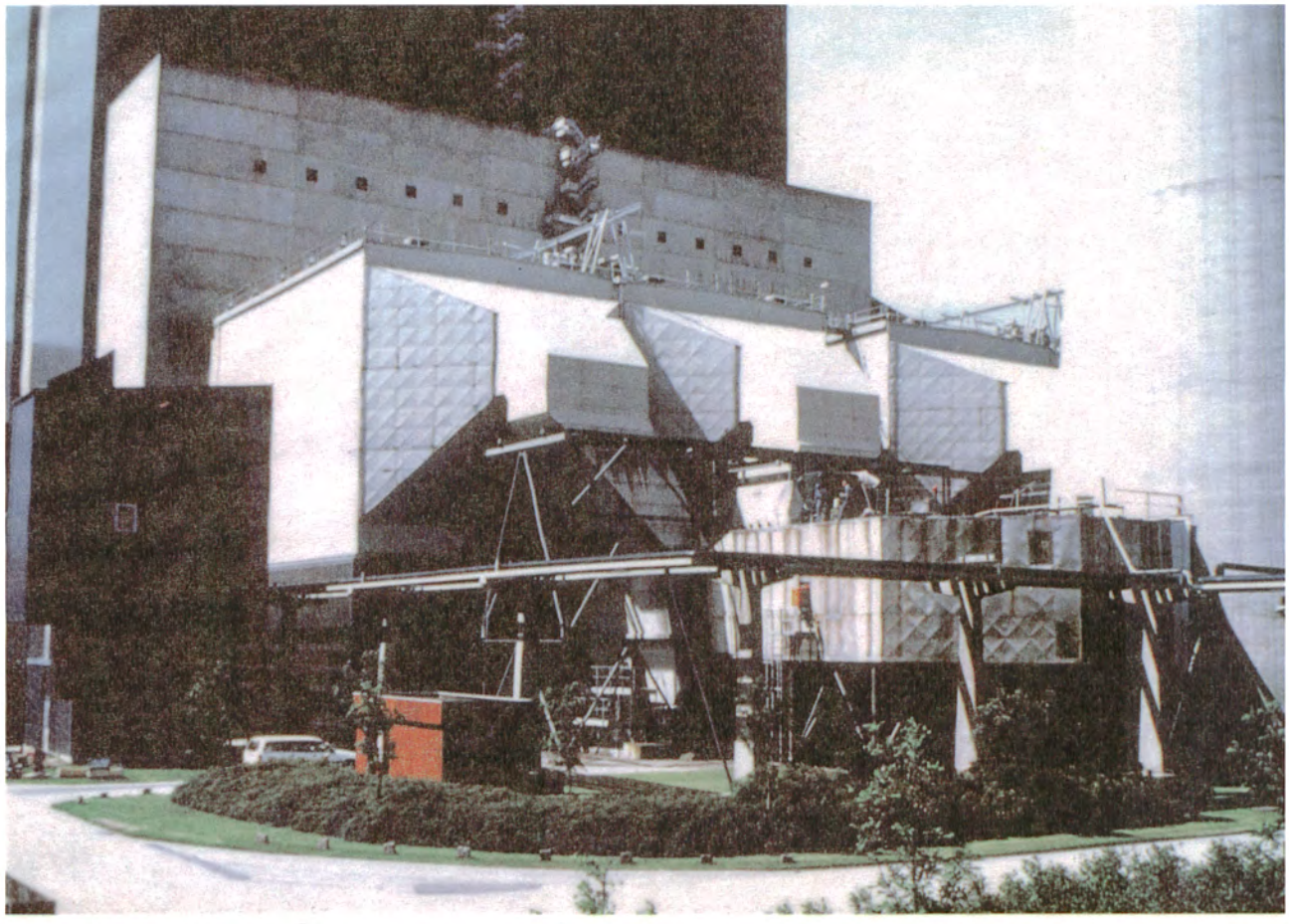

Plate 1. Field installation of an ESP.

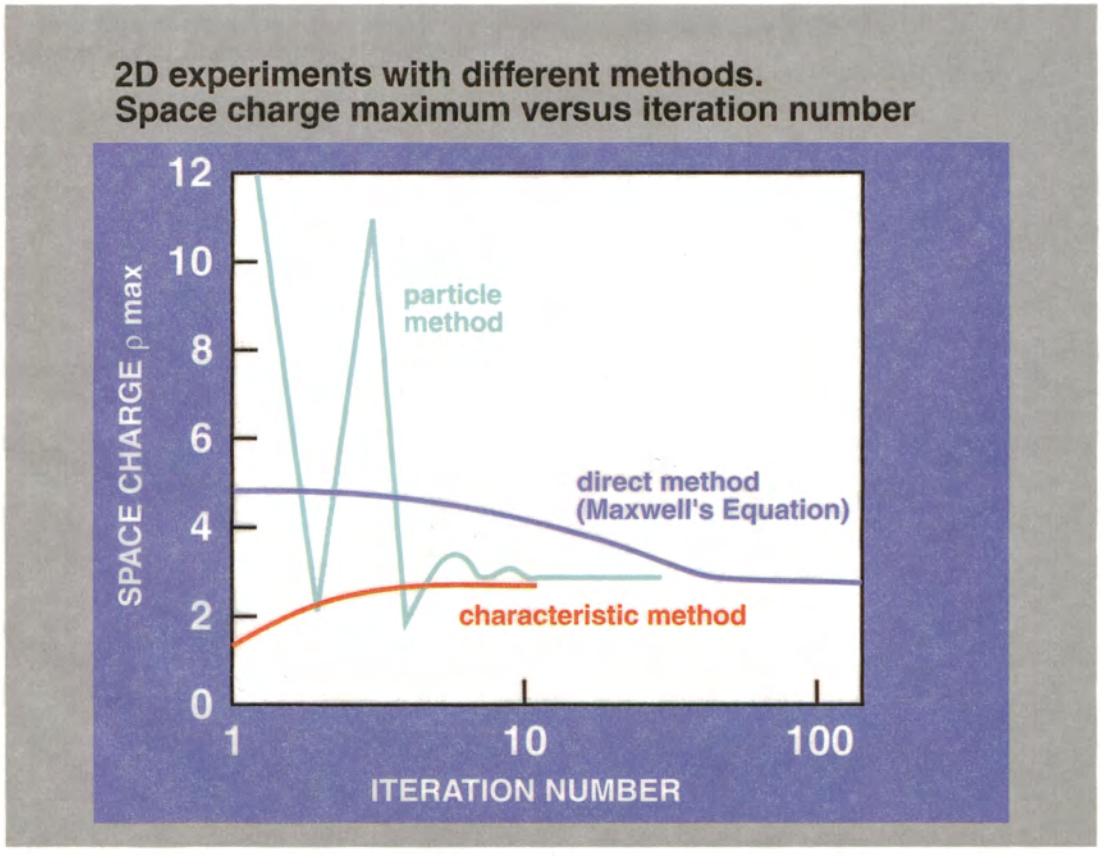

Plate 2. Comparison of different methods for the computation of the space charge distribution. Evolution of space charge maximum versus iteration number.

boundaries. For the implementation of the fluid solvers (FLOW) a data structure has been introduced, where each block is surrounded by a so-called halo, i.e., blown up by one cell. These halo cells overlap the internal block boundaries into the neighbour block. Three connectivity matrices are provided for the communication at block boundary surface points, at halo-cells and halo-points. The topology of the arbitrarily composed mesh blocks is thereby automatically derived by the usage of efficient search algorithms [4]. However, segmentation of block surface patches (for example two blocks connected to one) is not supported yet but will be introduced upon demand. This data structure is supposed to be generic in the sense that a smooth transition of space operators can be guaranteed for any kind of discrete scheme using stencils which connect neighbouring points or cells. Similar techniques have been successfully applied for the communication inside the iteration cycles of CFD-related numerical schemes on structured and unstructured domain split mesh topologies. A more recent issue for partitioning the space discretization is not only the enhanced flexibility in mesh generation but the natural route to map the algorithms onto distributed memory architectures which has once again become popular. The data structure is already designed for the straightforward communication via a message-passing paradigm.

3. Computation of the Electric Field Properties

Space charges are produced in an ESP first by the flow of ions from the discharge zone at the corona electrode to the grounded metal walls, and second by the movement of charged particles—the latter effect being much smaller. Three different methods have been investigated for the computation of self-consistent solutions of the charge density and electric field distribution: (1) the direct solution of the Maxwell's equation, (2) the computation of the charge density distribution by a particle pushing method and (3) the backward integration by a characteristics method. Although all three methods provide the same result, the third one is the most precise and efficient (Plate 2) and therefore is considered to be the method of choice. The procedure implemented for 2-D as well as for 3-D discretizations is as follows: at each mesh point the field line through this point is tracked back to the high voltage boundary at the rim of the active discharge region (each field line has an origin in a high voltage boundary), from where the integration toward the mesh point is started. In complicated multi-domain meshes, a sophisticated book-keeping takes care for the transition between internal block boundaries. Once the space charge has been determined the electrical potential is calculated solving the corresponding Poisson equation by using the ASTRID system [2]. The electrical field and the current density can be derived straightforward from this potential. Plate 3 illustrates an example for a 3-D configuration consisting of a channel and two spiral electrodes. This result exhibits a remarkable correlation of the current distribution with the different oriented spiral electrodes.

4. Model for the Flow Field

The general mathematical description of the gas flow is given by the Navier-Stokes equations where, for the flow condition in an ESP, appropriate turbulence models will have to be considered as well. Currently, the flow is simulated by using the system of Euler equations, which constitutes the most complete description when neglecting viscous effects. However, since a Navier-Stokes approximation can be derived by adding operators which discretize the shear stress terms, in principal the methods developed for the Euler equations can readily be extended to solve the more general Navier-Stokes equations. CFD modules that solve the set of Euler equations have been implemented into the PE^{2}AR environment for 2-D as well as 3-D flow simulations. The multi-disciplinary nature of the problem is reflected by additional source-terms for momentum and energy in the basic equations. Their magnitude depends on the electric field, the space charge, the particle charge and the relative motion of the particle with respect to the flow. The influence of the particle movement on the gas flow (Stokes forces) is not considered so far, but the coupling of the flow equations to the electric field properties is realized.

A two-dimensional model geometry bounded by two plane plates and with corona wires in the center plane has been considered. At conditions with low gas velocity and high electrical current (high electrohydrodynamic number) vortices form between the wires and the plates, driven by the so-called ionic wind. They are generated by the volume force resulting from the electric field multiplied by the space charge density. The potential together with the space charge is solved using the ASTRID system and the charge density distribution is calculated by the above described characteristic method. A simulation of the time evolution for the vorticity formation in a closed cell (no inflow velocity) has been carried out with a numerical finite volume Euler method. The resulting time constant to achieve a steady state (0.1s) is in good agreement with an integral valuation considering the equilibrium of electrostatic volume forces and momentum in the flow field [5], the induced velocity mean value for typical arrangements is in the order of 1 m/s. The time for the formation of rotation is assumed to be independent of the magnitude of the incoming flow.

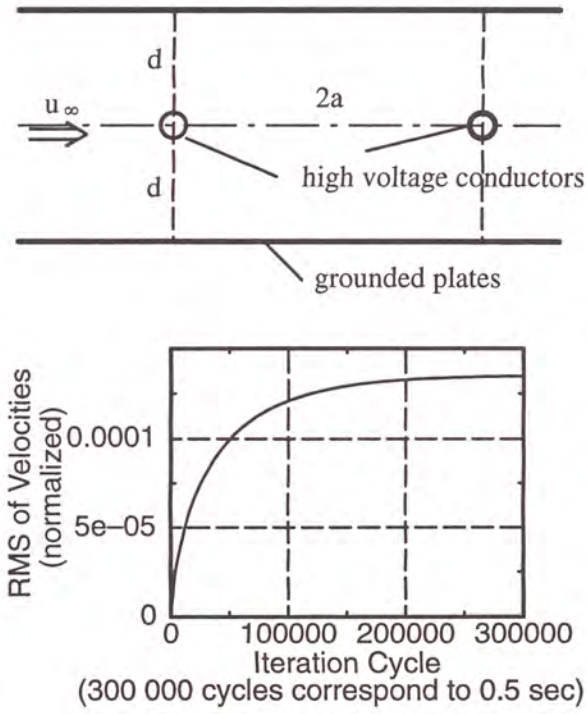

Figure 2. Definition of the considered plane two plate geometry with conductors and RMS of velocity for the formation of vortices in a fluid cell configuration: $u_\infty=0$.

Two distinct models have been applied to solve the fluid equations together with the electrical forces. The first one solves the compressible Euler equations in a time-accurate iteration process (Figure 2), whereas in a second model the incompressible equations with added artificial compressibility are solved by using the same numerical scheme with a pseudo-time iteration [6,7,8]. A large number of iteration-steps is needed for the time-accurate simulation of the gas-dynamic equations. This reflects the physical stiffness of the problem, i.e., the physical time-constant differs much from the time-step limit imposed by the explicit method which corresponds to the propagation of a pressure wave in the given mesh. Such numerical problems are reported by different researchers for the computation of gas-flows at low Mach-number. In such cases incompressible models are more efficient, if they are able to solve the physical problem adequately. The structure of vortices computed with the incompressible method is exhibited in (Figure 3).

5. Model for the Particle Movement

The models for gas-particle flows can be categorized according to coupling of the two phases and according to the approach. The assumption of one-way coupling neglects the reaction of the gas due to particle motion. These models require the specification of the flow field and particle trajectories are calculated by integrating the particle motion equations as the particles proceed through the flow field. Interactive coupling in which the mutual effects of both the particles and gas are included is referred to as two-way coupling. The already mentioned approach is distinguished according to the treatment of the multi-phase flow, which can be done again by calculating the trajectories and treating the particles as sources of mass, momentum and energy (Lagrangian model). The second approach solves the flow field on the basis of a multi-fluid model with distinct bulk densities or volume fractions for the different phases (Eulerian model), where no particle pressure exists for the dilute particle phase. In fact, the particle cloud is analogous to a compressible fluid without equation of state.

The two approaches mentioned above have both their inherent advantages and disadvantages in treating dilute gas-particle flows. In an ESP the particles first move with the velocity of the conveying phase. They get some amount of charge and their path becomes distinct from the flow field. The particle flow is currently simulated by a trajectory method, where a specific charging model has been implemented into an already existing ASTRID module for particle pushing [9].

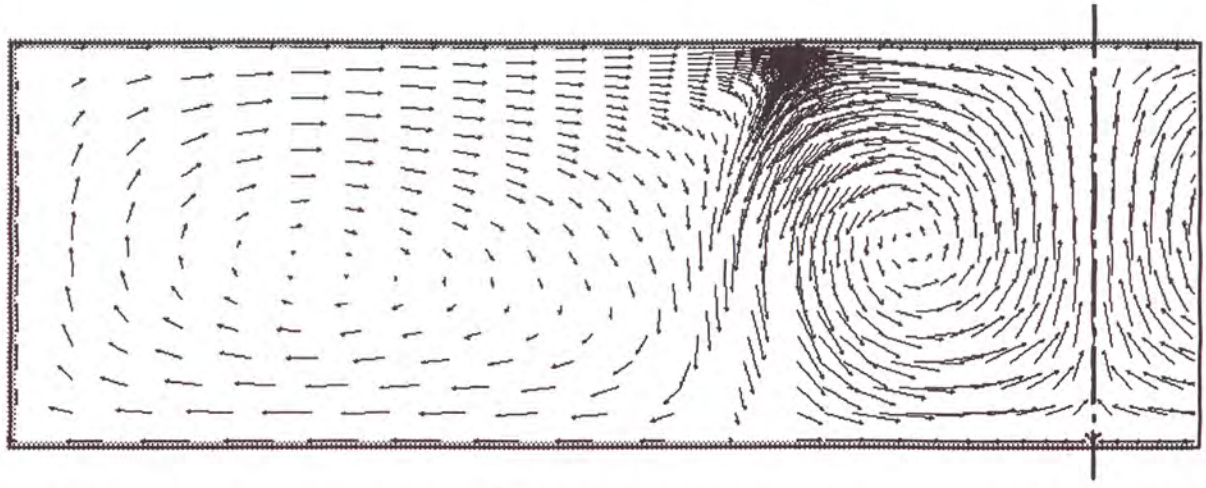

Figure 3. Counter-rotating vortices in a plane fluid cell configuration with conductors generated by the electric field forces, so-called ionic wind.

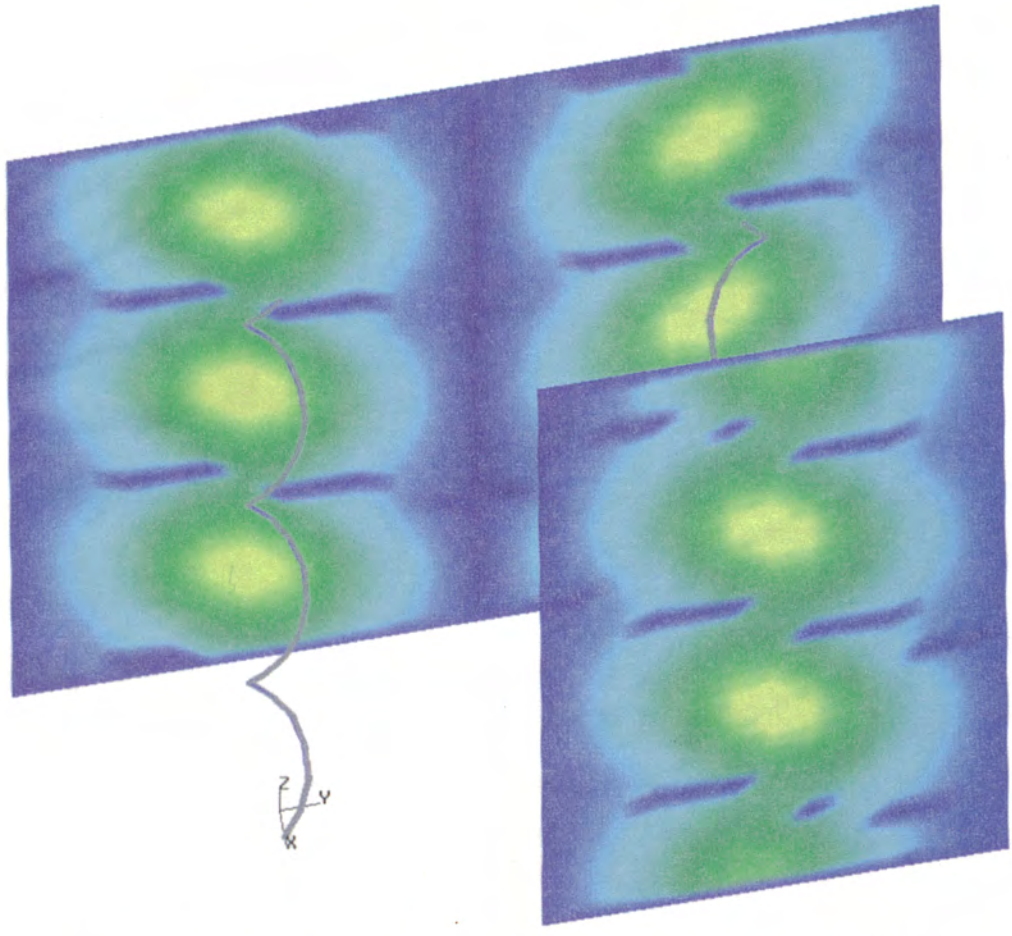

Plate 3. Current distribution on the grounded plates for a configuration with two spiral electrodes of different orientation.

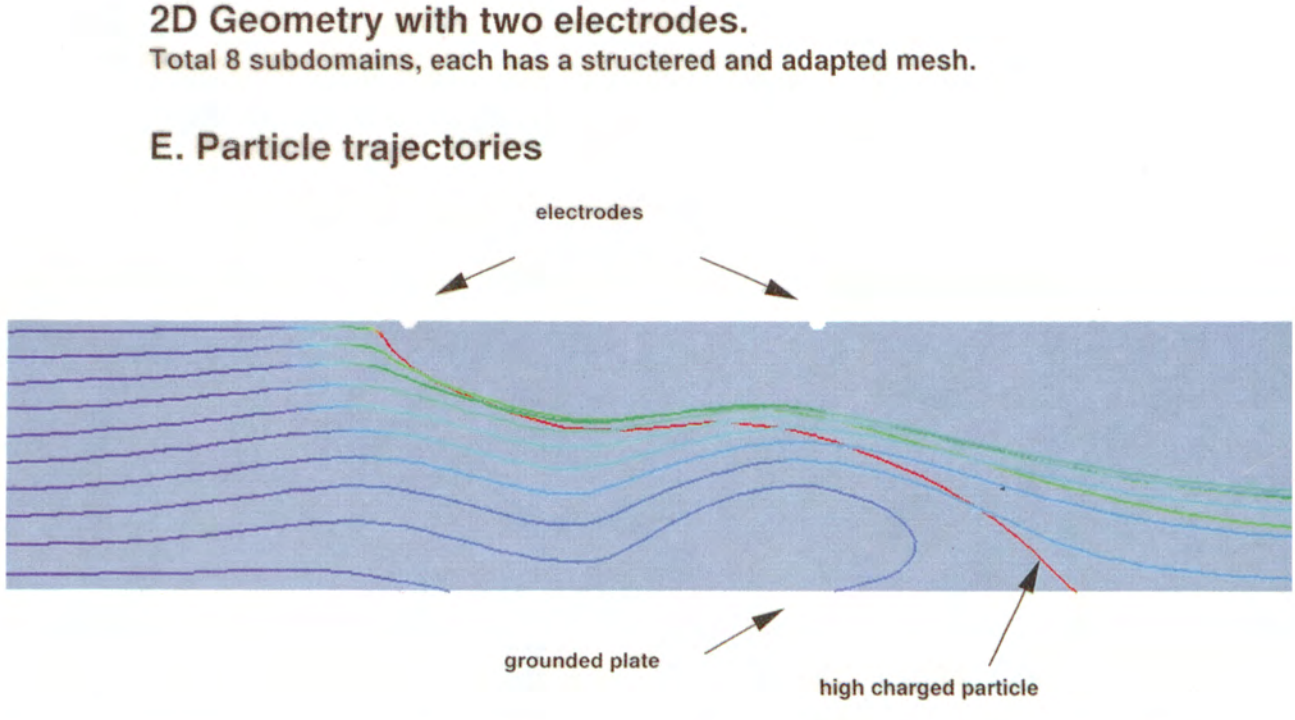

Plate 4. Trajectories of particles moving through a plane two plate configuration. Particles passing the electrode with small distance receive higher charge than those further away.

An example is given in Plate 4 where the particles passing the discharge electrode with small distance receive higher charge loading than the particles further away.

6. Conclusions

The development of a computational model for the simulation of an ESP is challenging because of the multi-disciplinary nature of the problem. Taking advantage of an environment called PE²AR has proved to be effective; modules developed by different researchers can be combined in a straightforward manner in addition to the usage of already existing programs. New modules implemented up until now comprise a method for providing two different models for the computation of the flow field together with electrostatic forces and a model for the particle movement, with self-consistent solutions of the charge density. In order to get a more complete theoretical idea of the physical behavior of an ESP, future development is necessary which will concentrate on the further refinement of the flow solution modules, on the coupling of the gas-flow with the dilute particle phase and on the investigation of further models for particle simulation, which is essential to develop a reliable additional new module for the dust layer.

Each computational model aims at providing a better understanding of the influence parameters for the corresponding technical facility. Investigations using the existing model have already been carried out with the purpose to optimize the electrical current distribution on the conductor plate. However, the reliability and accuracy of the method incorporated in an optimization strategy is demanding and the CPU-time requirement for performing a large number of optimization cycles is a limiting factor. Accordingly, much care has been taken by coding the recently implemented modules in order to take advantage of high performance computational platforms; i.e. on the SX-3 about 600 MFLOPS have been achieved for the CHARGE module and about 1.2 GFLOPS for the flow solver module. Finally, the target machines for the whole integrated application will range from workstations, over todays vector-supercomputers to future massive parallel and distributed shared memory platforms.

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JOINT CSCS-ETH/NEC HIGH-PERFORMANCE COMPUTING SOFTWARE DEVELOPMENT CENTER: FIRST RESULTS

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1. Introduction

Last year's CSCS annual report summarized the goals and objectives of the Joint CSCS-ETH/NEC Collaboration in Parallel Processing [1]; this ongoing project, comprised of ten researchers, is developing the integrated tool environment *Annai* and working on applications and algorithms for DMPPs. Most of these researchers began work in the fall of 1993, and therefore in our last report we could not go far beyond presenting tool design objectives and summarizing a target application suite.

In this report we describe first results achieved in 1994 while working towards our main goal: *turning massively parallel systems into practical tools*. *Annai* is being developed as a series of prototypes which permits our application group to use early software releases, to evaluate the tools and provide feedback, and to propose functional enhancements for inclusion in future prototypes. Although a common objective for tools and applications is portability, our main current development platform is a 128 processor NEC Cenju-3; this MIPS 4400-based distributed-memory parallel processor (DMPP) was installed at CSCS in July 1994. This report describes the functionality of *Annai*'s latest prototype and summarizes benchmark results of selected applications running in parallel on the Cenju-3.

2. The Tool Environment *Annai*

Three components within our tool environment *Annai* share a common user interface (UI):

a parallelization support tool (PST),
a parallel debugging tool (PDT) and
a performance monitor and analyzer (PMA).

The integrated environment accepts high-level extended HPF programs and low-level MPI code. PST acts mainly as a compiler for both paradigms. PMA and PDT are designed with the same philosophy, i.e., it is possible for the user to obtain information at different levels of abstraction. For ample details on PMA, PST and PDT we refer to [2], [3] and [4] respectively.

2.1 Parallelization Support Tool (PST)

The main objective of PST is to provide a higher-level programming interface than basic message-passing. HPF is well-suited for programming applications requiring highly structured computations but it lacks support for the parallelization of unstructured computations. We have shown in our previous work that for the efficient parallelization of such applications, a high-level language must also include constructs to dynamically distribute data and control flow and as a consequence the compiler must be able to analyze communication patterns at run-time.

The run-time analysis of PST is based on the *dynamic data consistency analysis* of the Oxygen compiler. We integrated this mechanism into an HPF compiler built by NEC Tokyo.

Using the HPF `EXTRINSIC` procedure interface, we extended this compiler to also feature run-time analysis and to support unstructured computations: in addition to the well known static `BLOCK` or `CYCLIC` data annotations, PST also allows dynamic user-defined distributions and explicit control-flow parallelization. Such user-defined data and loop distributions can be defined for instance by mapping-functions or mapping-arrays, the former being slow but memory efficient, and the latter fast but expensive in terms of memory overhead. Our application developers are currently designing the PLUMP library [5] on top of PST, for parallelizing applications based on unstructured meshes. To support PLUMP, we have added `BLOCK_GENERAL` distributions to PST. That is, arrays can be partitioned into contiguous sections with different strides on each processor.

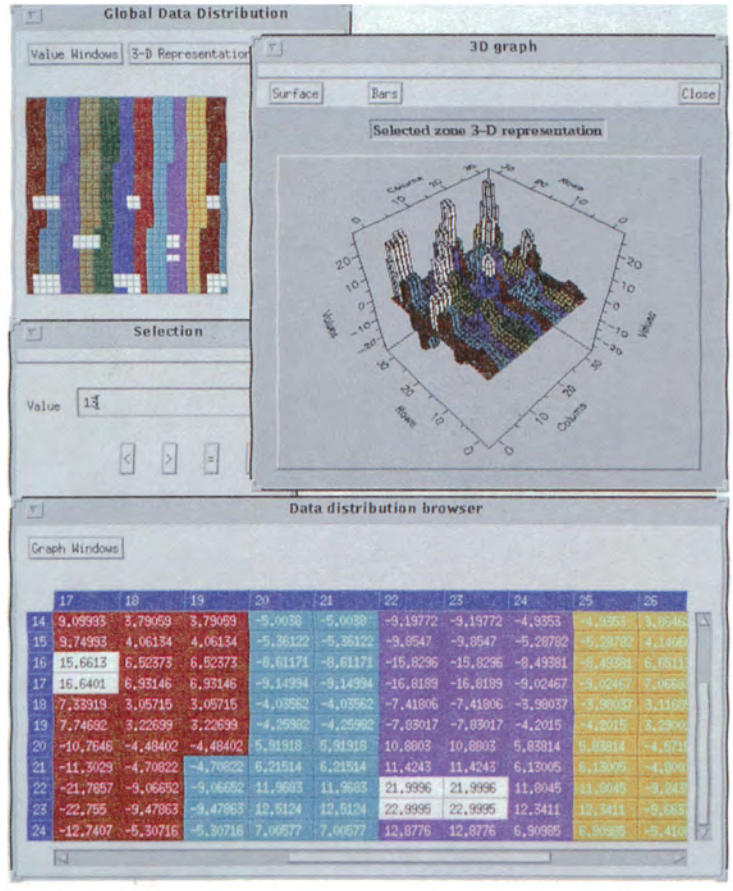

Plate 1. PDT numerical and 3-D distributed data displays. Coloring is used to distinguish PEs, and data values above 13.0 have been highlighted.

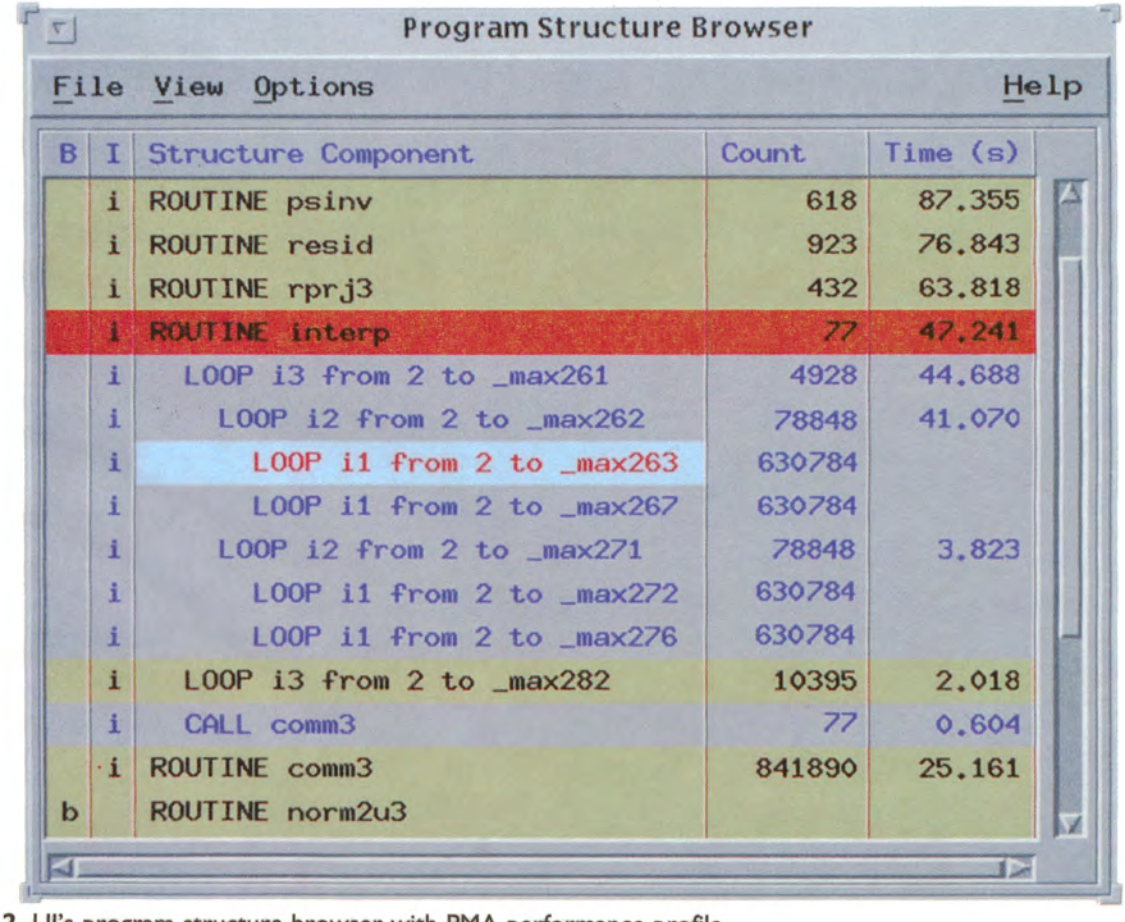

Plate 2. UI's program structure browser with PMA performance profile.

2.2 Parallel Debugging Tool (PDT)

A global breakpoint can be set on all PEs executing the parallel program. When a breakpoint is locally hit on any PE, the host coordinates global interruption of all participating PEs. Control is then given to the user who can inspect the state (stack, data segment and variables) of each individual process. Program exceptions are handled as global breakpoints. The mechanism to stop the machine when a global breakpoint has been reached is also used when the user wants to stop or terminate a program. When a parallel program is globally stopped, PDT automatically checks for deadlocks and allows display of distributed variables.

PST guarantees generation of deadlock and race-free parallel programs from HPF sources. As soon as the user mixes data-parallel and message-passing paradigms, both deadlocks and non-determinism due to races may be introduced. Race conditions may be non-intended and should then be regarded as programming error, or they may have been introduced by the programmer intentionally for improved performance.

PDT detects deadlocks at run-time by analyzing local processor stacks for cycle-detection in the global communication pattern. We have instrumented our MPI library to allow for race detection and deterministic replay. That is, a user can replay the order of communication events of a first program execution and inspect the program state reliably.

Plate 1 shows how PDT displays both distributed data values and locations for a PST `BLOCK_GENERAL` distribution.

2.3 Performance Monitor and Analyzer (PMA)

PMA provides facilities for monitoring and tuning of parallel applications, supporting high-level HPF/PST programs and low-level message-passing programs based on MPI. Initially, PMA is used to configure program instrumentation, ensuring that the desired level of information is collected with minimal intrusiveness. PMA uses the integrated facilities of the UI program source and structure browsers to select and mark regions which have instrumentation dynamically configured into the loaded (and possibly running) executable. Subsequently, the information collected during program execution is interpreted by PMA for performance analysis and visualization. Targeted understanding and tuning is supported via directed user interaction, selecting critical routines from overall performance profiles for localized investigation right down to the detail of underlying message-passing events and additional memory utilization overheads. In Plate 2 we show an example of how a performance profile of PMA can be depicted close to the original program source structure in UI's *program structure browser*. Program performance can be monitored throughout its execution by requesting updates at intermediate stages, when the collected information may be processed using the parallel computing system itself. Alternatively, after execution has completed, performance profiles can be analyzed off-line and compared with previously stored versions.

2.4 User Interface (UI)

The UI currently supports browsing through program source files, selecting break-points and checkpoints, invoking of different compilers (i.e., C, Fortran 77, and PST, with automatic selection of appropriate compilation flags and libraries). It allows to invoke and manage PDT and PMA from the one unifying interface. The UI has been enhanced by an interactive program structure browser (see also Plate 2) which displays the important components of the program source structure, and allows entries to be annotated with performance metrics furnished by PMA and debugging information furnished by PDT.

3. Application and Algorithms

Our work on applications and algorithms during 1994 can be split in three categories: (1) parallelization of standard benchmarks and performance measurements on the Cenju-3, (2) parallelization of some of the applications listed in our application suite document [6] and (3) design and library-based implementation of parallel algorithms. In the frame of this report we can not detail all of the work performed in each of the three categories. Instead we enlist the names of each of the software packages and then describe the parallelization of two selected applications. For more details on any benchmark, application or library the interested reader is kindly asked to contact W. Sawyer. Most of the work has been documented in a variety of technical notes, reports and publications.

As benchmarks we first considered the NAS benchmark kernels Embarrassingly Parallel (EP), Block Tridiagonal (BT), Multigrid (MG), Conjugate Gradient (CG), Fast Fourier Transform (FT) and Integer Sort (IS). Second a benchmark from

an industrial collaborator (Electricité de France) was parallelized and used to evaluate the performance of the NEC Cenju-3. Parallelization of the following application codes is either completed or still ongoing: *Molekel*, *tJ-Model*, LASO, *Raytran*, *ME*, *TBMD*, and *SOLIDIS*. Finally parallel algorithms were collected in the libraries KSM, PRNG, PLUMP (see also [5]) and BLACS.

For the remainder of this section we will describe results collected with two scientific example applications which come from developers in and around CSCS: *Molekel* for molecular visualization and *tJ-Model* for superconductivity.

3.1 Molekel

Molekel is a 3-D molecular graphics package for the interactive visual representation of molecular structures and properties [7]. *Molekel* contains various data-interfaces to external electronic structure calculation packages such as *Gaussian*, *AMOSS*, *deMon*, etc.

In order to generate iso-surfaces of electronic properties such as the electron density or the spin-density, *Molekel* calculates these properties at each point of a predefined grid. If this grid is large and the associated molecular structure very complex, the process of calculating these values may be very computation-intensive. Because the appropriate algorithms involve many complex scalar memory-operations using dynamic data structures, processing the computation-intensive parts of *Molekel* on a vector-computer will not improve performance considerably.

PEs	Total time [s]	Calculation time [s]	Speedup
1	14182	14044	1.00
2	7165	7025	1.97
4	3849	3708	3.68
8	2045	1988	6.93
16	1286	1129	11.02
32	828	671	17.13
64	587	430	24.16

Table 1. Performance times and speedup of Molekel exponential evaluation on the Cenju-3.

PEs/ # Samples per PE	Calculation time [s]	Speedup
1/128	4060	1.00
2/64	2212	1.83
4/32	1145	3.54
8/16	722	5.63
16/8	391	10.40
32/4	217	22.10
64/2	137	30.00
128/1	96	42.30

Table 2. Total time, calculation time and speedup of the *tj-Model* code.

On the other hand the parallel implementation of this algorithm is straightforward. Provided all processing elements (PE) have the same input information, the calculation of any point in the lattice is independent of all others, making the problem "embarrassingly" parallel.

Results

As a test case we consider the Carbon-60 (C_{60}) molecule in a lattice containing 68 x 75 x 68 points. Table 1 illustrates the time required to evaluate the electron density at each grid point for different numbers of processors. Since the grid is decomposed into slices, the load is not distributed evenly for higher number of processors (i.e., some processors have twice as much calculation to perform), and the speedup for larger number of processors degrades accordingly.

3.2 tJ-Model

The *tJ-Model* code investigates the region of superconductivity in the phase diagram of the 2-D *tJ* model—the simplest model to describe strongly correlated electrons—with the help of a modified variational Monte-Carlo (VMC) method [8]. The *tJ*-Model has various phases with different *broken* symmetries. If enough information about the symmetries of the ground-states is known, variational wave functions can be constructed to model them. At small hole dopings, the energy values of these phases will be close to each other, such that the energy differences are comparable to the errors introduced by the use of modified variational wave functions. Therefore the regions of stability of the various phases in the phase diagram can only be estimated qualitatively. By combining a generalized Lanczos scheme with the variational Monte-Carlo method it is possible to reduce the bias in the choice of the wave functions and optimize the short- and long-range properties. Since this implementation considers larger problem sizes than existing codes, the finite-size effects are kept small.

The *tJ-Model* is parallelized by executing the same program on each processor with a different initial random seed. The total number of random samples is kept constant (in our benchmark, 128 samples were generated).

Results

As shown in Table 2, the *tJ-Model* exhibits good speedup even for few sampling steps and for large numbers of processors. Since the random-path, which is generated by means of the Metropolis algorithm, differs from one processor to another we get also different "walking times", and thus execution times. The speedup factor is taken with respect to the slowest process.

4. Future Work

The collaboration is an ongoing project and, during the next year, both tools and applications will be subject to frequent modifications, enhancements and additions. We will improve the existing tool prototypes and their robustness, investigate possibilities for increasing tool "intelligence", tackle the port to platforms different in architecture to the Cenju-3 (in particular platforms with additional hardware supporting shared memory and with vector processing nodes, such as the NEC SX-4), pursue further third-party collaborations in the development of applications, add functionality to existing libraries and implement new ones to enlarge the spectrum of supported applications, and we will study the usefulness and feasibility of a knowledge-based application development tool to assist the user in choosing appropriate library routines.

Acknowledgements

The work on *Annai* has largely benefited from the help of the software development group headed by T. Nakata at NEC Central Research Laboratory in Tokyo. We also wish to thank former project members G. Jost and E. de Sturler and all the internal and external collaborators who contributed to the development of applications; in particular P. Flükiger, E. Heeb, and C. Stern who were involved in the parallelization of *Molekel* and *tJ-Model*. Many contributions to tools and applications are due to the participants of the 1994 CSCS SSIP, namely I. Beg, T. Bütikofer, M. Guggisberg, U. Krishnaswamy, E. La Cognata, M. Meehan, P. Przybyszewski, T. Schrøder, T. Toupin and W. Ling.

References:

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HUMAN CAPITAL & MOBILITY PROGRAM: INTERACTIVE IMAGE PROCESSING AND SYNTHESIS ON INNOVATIVE COMPUTER ARCHITECTURES *NETWORK*

Involved Persons:
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M. Hohenadel ..... a
U. Meyer ..... a
I. Pontiggia ..... a
Organizations:
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Center for Novel Computing, Victoria University of Manchester (U.K.)
CERFACS (France)
CRIL Ingénierie (France)
Dipartimento di Scienze dell'Informazione, Università di Milano (Italy)
Institut Gaspard-Monge, Université de Marne-la-Vallée (France)
ISEI Institute, JRC (Italy)
LABEIN (Spain)
RAL (U.K.)
Funding Sources:
BBW (KWF)
CSCS
European Union (other partners)
Duration:
September 1993–March 1995

Human Capital & Mobility is a large program initiated by the Commission of the European Communities, Direction General XII. It consists of so-called *networks* that bring together research centers with common interests to foster technical experiments as well as knowledge and experience transfer among them by exchanging researchers for the purpose of collaborating in research activities.

The network of *Interactive Image Processing and Synthesis on Innovative Computer Architectures* aims to develop a common understanding of the problems of image data analysis and manipulation, to exchange software tools and systems, to exchange expertise, and to experiment with each other's approach and methods on different hardware platforms (and particularly parallel computers) and in different application areas. In the medium term it is expected that this will allow identification and development, in collaboration with others, of common tools and environments which can be used in a wide variety of applications. In the established network, these include computational fluid dynamics, satellite and medical image processing, image data compression, realistic image synthesis, visualizing complex 3-D data (CAD), molecular modeling and graphics.

The original project duration was September 1993–September 1994. The startup phases, however, took more time than planned. A six-month extension was granted by the Commission to compensate for delays. The official project end is now March 1995.

Partners

The ISEI (JRC) and the CSCS have a principal collaboration defined by a bilateral contract. Both organizations are partners in the network of *Interactive Image Processing and Synthesis on Innovative Computer Architectures* of the Human Capital & Mobility Program. The entire network consists of the following nine partners:

- Centre de Recherche et de Formation Avancée au Calcul Scientifique (CERFACS), Toulouse (France)
- Dipartimento di Scienze dell'Informazione, Università degli studi di Milano, Milano (Italy)
- Center for Novel Computing, Victoria University of Manchester (U.K.)
- Institut Gaspard-Monge, Université de Marne-la-Vallée, (France)*
- Rutherford Appleton Laboratory (RAL), Chilton, Didcot (U.K.)
- Centro de Investigación Tecnológica, LABEIN, Bilbao (Spain)
- CRIL Ingénierie, Toulouse (France)
- ISEI Institute, Joint Research Centre (JRC), Ispra (Italy)
- CSCS, Manno (Switzerland).

* This research group was previously located at Laboratoire d'Informatique de Besançon, Université de Franche-Comté, Besançon (France).

CERFACS is the main contractor to the Commission of the European Communities (CEC). The other partners are subcontracted by CERFACS. A special bilateral contract exists between JRC Ispra and CSCS.

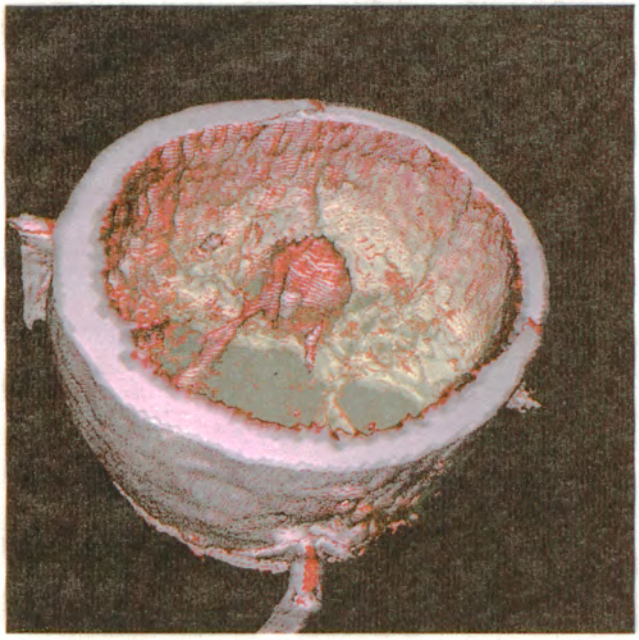

Plate 1a. 512x512/24 bit (768 KB) image of a cranial tumour, generated by X-EVA software from the University of Milan.

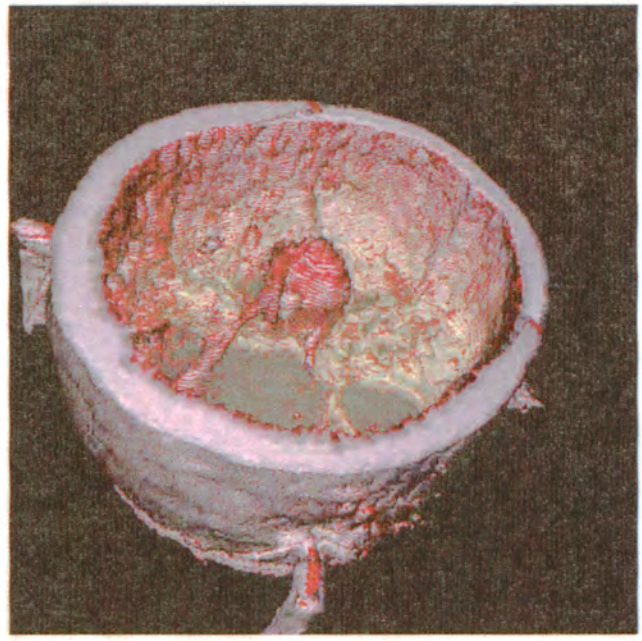

Plate 1b. Image reconstructed after compression by Undine. Compression Ratio was 23 (33 KB).

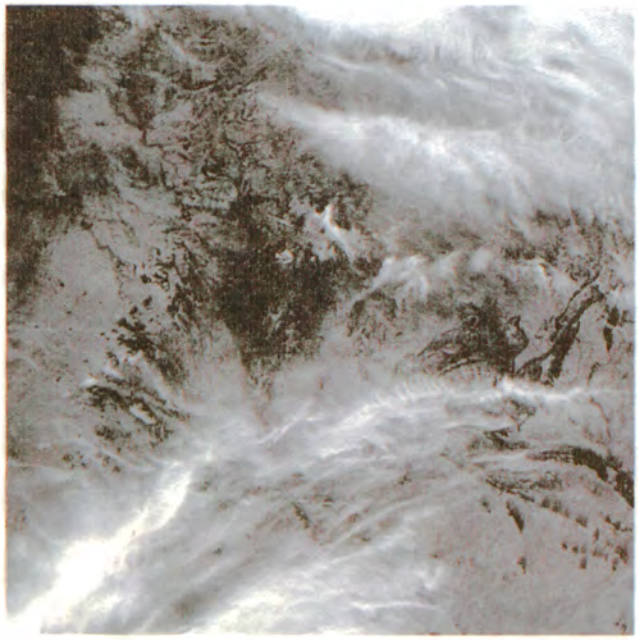

Plate 2a. 512x512/8 bit (256 KB) image of Himalaya mountains captured by the ERS-1 satellite. This ATSR image is coming from RAL.

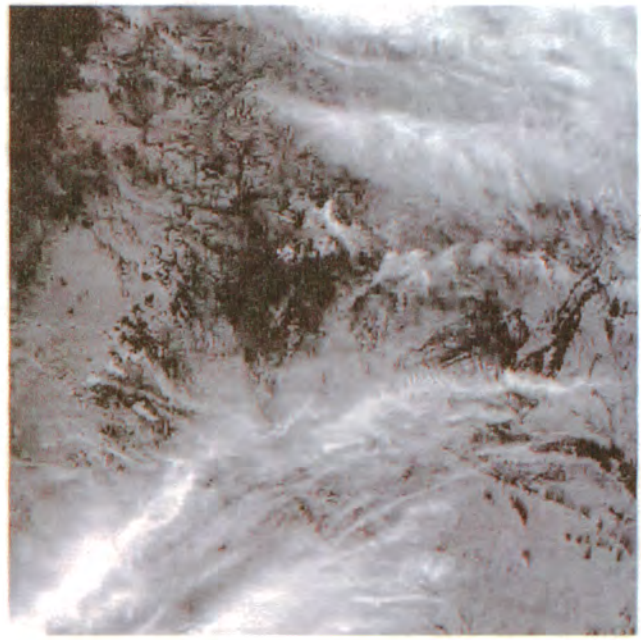

Plate 2b. Image reconstructed after compression by Undine. Compression Ratio was 26 (10 KB).

Organization

The internal organization of the network was defined in an early plenary meeting. Three working groups have been formed to bring together partners with common interests and experience. Although there is overlap between groups, the three central working groups, main themes, and participating partners are:

1. Image manipulation working group

- image compression algorithms
- image processing
- remote sensing analysis

Active partners: CRIL, RAL, Università di Milano, JRC Ispra, and CSCS.

2. Visualization of numerical analysis working group

- computational fluid dynamics visualization
- electromagnetism visualization
- finite element methods
- molecular graphics
- graphical user interfaces

Active partners: RAL, LABEIN, CERFACS, Victoria University of Manchester, and CSCS.

3. image synthesis working group

- radiosity and ray-tracing algorithms
- volume visualization, medical imaging
- photorealism, CAD/modeling

Active partners: Université de Marne-la-Vallée, JRC Ispra, Victoria University of Manchester, and Università di Milano.

Activities

CSCS participated primarily in first two working groups but has been working in the following areas: image compression, remote sensing analysis, scientific visualization and graphical user interfaces, and the development of an image processing and synthesis algorithms library.

1. Image Compression/Image Manipulation

Activities in this working group (subpart image compression/manipulation) lead to enhanced image compression tools and a report on remote sensing applications. Algorithms that are similar to JPEG in their structure but use other fast transforms such as the wavelet transform have been developed. M. Hohenadel (CSCS but previously at JRC Ispra) worked on a new implementation of the wavelet-based image compression algorithm developed at JRC Ispra. The first tests were very promising. With greyscale test images compression factors well over 20 have been achieved with extremely low loss of quality. In a further step the algorithm will be applied to various data provided by other partners. Also, the use of such kind of algorithms for remote visualization will be studied.

M. Datcu (CSCS visiting researcher from DLR–Deutsche Forschungsanstalt für Luft- und Raumfahr) has been working on remote sensing applications dealing with the analysis of stochastically multi-dimensional processes using multi-resolution and hierarchic representations. Again, wavelet-based techniques have been used.

2. Image Processing and Synthesis Algorithms Library

The image processing and synthesis algorithms library is intended to provide an environment on innovative computer architectures to implement or port the algorithms developed in the other parts of the project and by other partners in the network. Domains that we deal with are volume visualization, image compression, and color correction. The PVM library, that provides a message-passing interface to a heterogeneous computer environment, has been chosen as the low level basis.

I. Pontiggia (CSCS) has been handling this part of the project. He successfully parallelized his color correction program and ported it to the PVM environment. The EVA volume visualization software (developed at Università degli Studi di Milano in the group of D. Marini) is almost completed. A fractal image compression program developed by the same group has been parallelized on the Cenju-3 during the 1994 SSIP (see page 25).

3. Scientific Visualization and Graphical User Interfaces

Activities in this working group resulted in graphical user interfaces for scientific visualization being enhanced or developed to make the scientists task easier. Special focus has been placed on the improved user-friendliness. If large data amounts have to be processed and analyzed, general purpose packages exhibit performance and space limitation problems. As a consequence, specialized packages, each with a different user-interface, have to be used. The goal of a common interface for visualization packages, at least within the same application area (computational chemistry to be specific), has been partially met. Another focus is on input generation tools that serve as interfaces to important simulation software packages. The same interface that is used to visualize simulation results should be enhanced with the appropriate functionality to setup simulation parameters, launch the calculation and retrieve the results.

One specific application area is molecular graphics. P. Flükiger (CSCS) extended his molecular graphics package *Molekel* with a prototype input generation tool for Gaussian90. Furthermore, a large portion of the porting to the Motif environment has been completed.

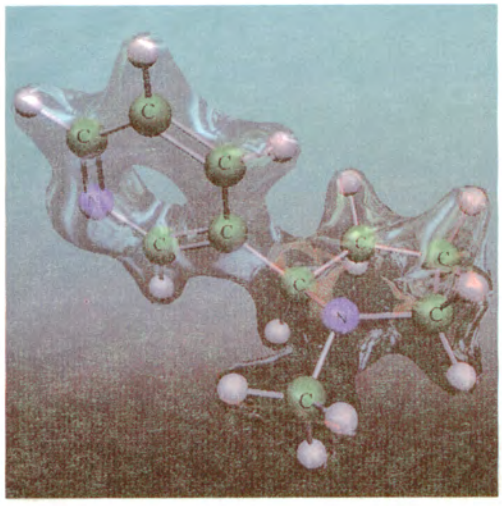

Plate 3a. 1024x1024/24 bit (3072 KB) image of nicotine molecule generated by Molekel software.

Plate 3b. Magnified.

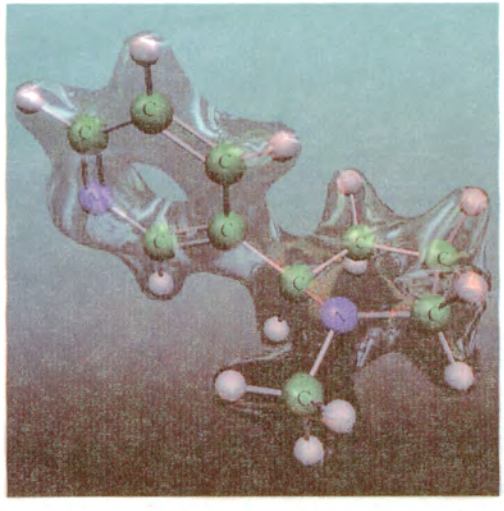

Plate 3c. Image reconstructed after compression by Undine. Compression Ratio was 119 (26 KB).

Plate 3d. Magnified.

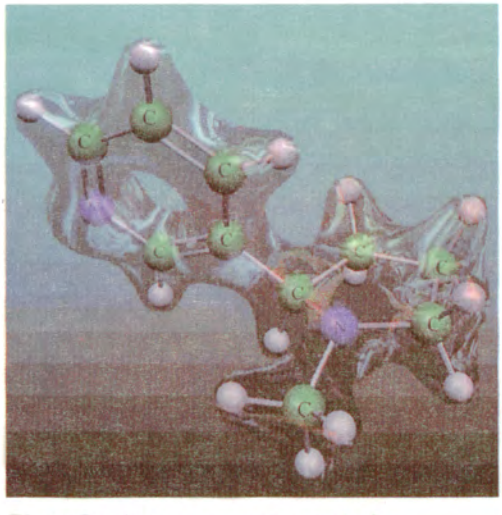

Plate 3e. Image reconstructed after compression by JPEG.
Compression Ratio was 119 (26 KB).

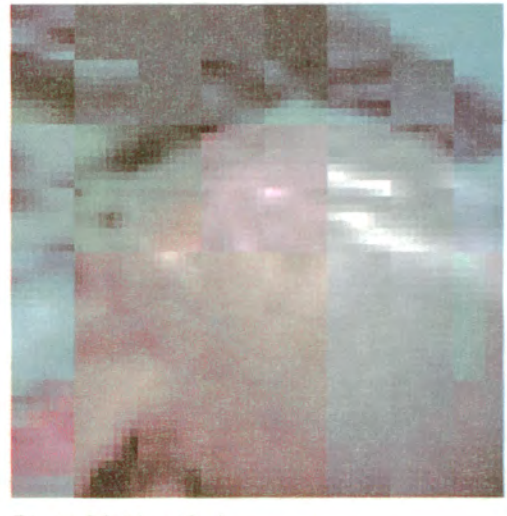

Plate 3f. Magnified.

USER-DRIVEN DEVELOPMENT OF A NOVEL PROGRAMMING ENVIRONMENT FOR DISTRIBUTED MEMORY PARALLEL PROCESSOR SYSTEMS

Involved Persons:
K.M. Decker ..... a
J.J. Dvorak ..... a
R.M. Rehmann ..... a
Organizations:
a CSCS
Funding Sources:
SNF
Duration:
March 1993–December 1995

1. Introduction

DMPPs are widely considered as an enabling technology for the future of high-performance computing. One of the advantages of DMPPs is their scalability to massive numbers of processors and, equally important, to huge memory sizes. Over the last few years, several DMPP systems became available as commercial products. An essential drawback of DMPPs is their difficult programmability, since the management of the address space is shifted either to the language or even the user level.

It is the goal of our research to develop a program development environment (PDE) for DMPPs oriented towards the application user's expectations (such as ease of use, relying on familiar terminology, achieving highest performance and best parallel efficiency), portability, scalability of resulting programs, protection of software development efforts, and adaptability and extensibility of the environment to changing needs [1]. To satisfy such high expectations, the PDE embodies a knowledge-based approach with application-oriented problem description formalisms and offers intensive guidance to the user. It makes the actual coding process transparent as far as desired, supports the protection of software development investments, and is adaptable to the user's needs.

Our approach towards intelligent programming environments for DMPP systems has been inspired by reflections about problem solving environments [2] and is founded on three methods: formal specification languages, methods from artificial intelligence, and automatic program synthesis techniques.

2. Methodology Overview

A programming environment with user support starting early in the program development process seems most appropriate [3]. The PDE covers important parts of the complete program development procedure, from problem specification and design up to—and including—code generation. Emphasis is placed on user interaction at a high level of abstraction, well above the level of standard programming languages.

The programming methodology supported by PDE consists of the following three steps:

1. problem-oriented specification using a formal language presented in a comfortable GUI;
2. interactive refinement and completion of the specification when this is necessary;
3. user-transparent generation of compilable program code depending on user' expertise level.

From the application user's point of view, the problem-oriented specification language formalism in step 1 is probably the most important ingredient of the methodology. It supports a declarative description of the problem in a user-oriented way, using a terminology which is inferred from the terms used in the user's problem domain, avoiding the jargon of computer science to a large extent. This strategy ensures that the programming methodology is readily managed by scientific users. If the problem is underspecified or cannot be described completely, interactive refinement and completion of the specification (step 2) is required. In these cases, interactive guidance becomes crucial.

The programming methodology relies fundamentally on the concept of *algorithmic skeletons*. See [4, 5] for more detail.

3. Results

3.1 A Programming Environment for Stencil-based Problems

To ease DMPP programming of applications in the class of stencil-based problems on n-dimensional grids, we have developed three PDE prototypes with successively enhanced functionality [1]. The stencil modeling programming assistant interface (SMPAI), realizes an interface to the PDE for this problem class, by providing complete support for the solution of, for instance, problems based on the finite difference method. The SMPAI supports a complete problem description. This means that once the problem has been described, there is no further user interaction required. Exploiting different knowledge bases and techniques from artificial intelligence, the PDE generates the compilable program code in a fully automatic fashion. Within the SMPAI, the user specifies the problem type, the geometry of the problem domain,

the size and dimensionality of the grids, the boundary condition for each physical boundary of the grid, the structure of a grid cell, the computational stencil, the numerical method, and the domain decomposition scheme.

We have successfully demonstrated that such a complex system can be built and that most of the design objectives have been realized: declarative, application-oriented problem description, software reuse, user transparent exploitation of parallelism including support for portability on the algorithmic level, complete abstraction from hardware issues, and scalability. Since the problem description in the SMPAI is in general complete, user guidance is of no relevance for this problem class.

Applications used to demonstrate that (beginning with a user-oriented declarative problem description) efficient and portable parallel code can be generated in a completely transparent way, include the restoration of gray-scale images and the solution of partial differential equations.

From the application user's point of view, the problem domain of stencil-based applications is of relatively low importance. This must be considered as a conceptual limitation of the SMPAI.

3.2 Towards Programming of General Data-parallel Problems

To qualitatively increase the usefulness and attractiveness of the PDE, our current research is concerned with a major step towards supporting the programming of real problems of practical interest for the scientific user community.

To achieve this goal, we follow a step-wise approach and successively narrow down the problem spectrum of interest to this community. First, we stick to the class of general data-parallel problems. Within this problem class, the initial focus is on problems expressed by means of linear algebra operations. The first prototype of the data modeling programming assistant interface (DMPAI) is currently under implementation. It extends the PDE with a programming environment for iterative solvers for general linear systems.

The problem class of iterative solvers for general linear systems has very different characteristics than the class of stencil-based problems: the problem description may be incomplete, problem realization may require more than one algorithmic module with a fixed parallel structure, and consequently, the careful design of data structures becomes crucial.

An essential part of the DMPAI is the underlying declarative problem specification language. Within the 1994 SSIP, BLIPS has been designed, and the corresponding parser has been implemented [6] (see also page 27). In addition, a prototype of a complete stand-alone system for BLIPS-based declarative programming of iterative, parallel solvers has been realized.

Since the problem description specified within the DMPAI may be incomplete, the PDE must be able to communicate with the user in order to resolve ambiguities. To achieve this, we have realized the intelligent skeleton programming environment (ISPE).

The ISPE is a collection of tools to support programming with a hierarchically organized collection of algorithmic skeletons. The ISPE operates in close interaction with PDE's knowledge and rule bases and heavily relies on user interaction in order to get the information needed. To cope with incomplete or underspecified problem descriptions, ISPE tools can handle the case when the automated reasoning stops before reaching a sufficiently elaborate solution, or when the user wants to add missing information. The user can also actively interrupt the reasoning process at any time. He can select partial solutions manually, or even step through the inference process guided by the expert system. This allows the user to become more and more involved in the programming process, if this is desired—an ability of general interest for expert programmers. In the case where there is no initial problem specification, the ISPE can also be used for interactive programming.

The ISPE contains a *skeleton viewer*, a *skeleton tree browser*, a *decision support tool*, and a *skeleton completion tool*.

4. Outlook

What are the next steps which we foresee towards simple usage of DMPPs with powerful novel programming environments? First of all, we will concentrate on improved programming environments for the class of data-parallel programs. We intend to successively relax the constraints currently imposed on the supported application spectrum. Second, formalization of the large amount of application knowledge is crucial to ensure the long-term success of these systems. Third, the supported application spectrum should be broadened further, and support for non-numerical problems should

be realized. The latter is crucial for commercial applications. Fourth, to fully realize the objective that the user should be able to become more and more involved in the programming process, we believe that our current system should be vertically and bi-directionally integrated with a tool environment like *Annai* [7]. Finally, another important topic which we believe should be addressed in the near future is teaching effective usage of DMPPs. Here we envisage machine-assisted learning realized in an enhanced version of our PDE.

Acknowledgement

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TIGHT-BINDING MOLECULAR DYNAMICS FOR LARGE-SCALE SIMULATIONS ON SEMICONDUCTOR MATERIALS

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Funding Sources:
Consiglio Nazionale delle Ricerche, Roma (Italy)
Fondation pour des Bourses d'Etudes Italo-Suisses
Duration:
January 1993–December 1995

The tight-binding molecular dynamics (TBMD) scheme was recently introduced to bypass some intrinsic deficiencies of classical molecular dynamics (MD) (like the relatively poor reliability and transferability to complex materials), and to reduce the computational workload that severely limits the application of first-principle MD to those large-scale problems which involve hundreds or thousands of atoms. Simulations involving such a huge number of particles are relevant to problems of paramount importance in materials science such as the physics of solid surfaces and interfaces; the structure, thermodynamics and kinematics of extended defects in semiconductors; the structural and electronic properties of polycrystalline and porous materials.

The basic idea of TBMD is that the quantum mechanical many-body nature of the interatomic forces is taken into account naturally through the computation of the electronic structure of the investigated sample by means of an empirical tight-binding (TB) Hamiltonian. Among the several appealing features of TBMD, it is worth mentioning its relative ease of implementation, the possibility of running TBMD simulations (up to few hundreds of particles) on workstations, and its high numerical efficiency.

During 1993 we have developed an optimized TBMD code for the NEC SX-3 supercomputer which was ported and tested in 1994. In particular we:

(i) carefully benchmarked the performances of our code as function of the mathematical library used for diagonalization of the TB matrix. EISPACK, ASL, NAG and LAPACK routines have been tested and we found that the later was the slightly more efficient one;
(ii) carefully avoided any bank conflicts which were as large as the 66% of the total CPU time of each run in the preliminary runs of the original release of the TBMD code;
(iii) vectorized most of the do-loops.

The corresponding speed of execution increased by about a factor 10 from the original release (the floating-point format was 64-bit wide, corresponding to the CRAY representation). The absolute best performance was obtained during a simulation operated on 512 silicon particles where, running on a single processor of NEC SX-3, we observed a sustained maximum speed of 1.66 GFLOPS with more than 98% of the operation vectorized, and less then 0.5% of CPU time lost in bank conflicts.

The resulting code is suitable for extensive simulations where up to several hundreds of particles are present. It is, however, intrinsically scaling as the cubic power of the number of particles (N). In order to bypass such a N-cube bottleneck, we have implemented (in collaboration with S. Goedecker, Cornell Theory Center, U.S.A.) a novel formulation of TBMD where the computational workload scales linearly with the number of atoms (O(N) method). This result allows for large-scale TBMD simulations on systems with unprecedented size even on serial computers. Similar results have been obtained by other groups, thus confirming the relevance of this problem to large-scale computations in materials science.

More interestingly, the new formulation has been parallelized in collaboration with R. Mastropietro (CSCS) and executed on the workstation cluster present at CSCS. The PVM language was used to master the parallelism. The efficiency of this parallel code was awarded the 1994 Gordon Bell Prize for the best price/performance ratio.

The present implementation of parallel TBMD makes affordable simulations on systems containing as many as several thousands particles and large-scale applications on problems of paramount importance in materials science.

In addition, we have started a new project aimed at parallelizing the TBMD code for massively-parallel computers in collaboration with W. Sawyer (CSCS). The key idea is to apply the concept of entry re-ordering of the TB matrix in order to keep the bandwidth of such a matrix (now stored in a band format) as small as possible. This, in turn, allows for a dramatic reduction of the interprocessor communications. The first step of this research line was carried out in the frame of the 1994 CSCS SSIP where I. Beg implemented the re-ordering process (see page 19).

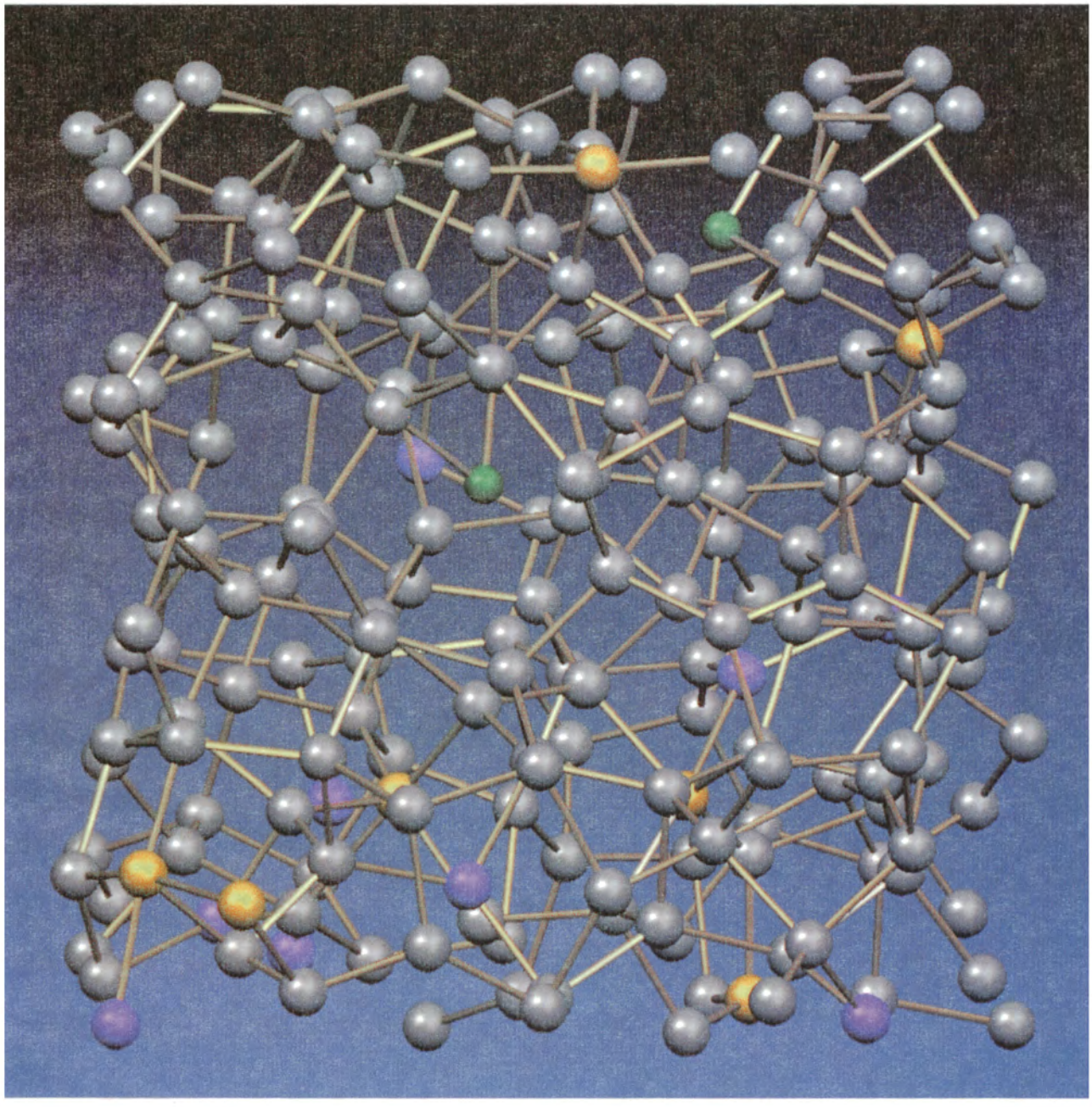

Plate 1. Three-dimensional view of the amorphous silicon networks resulting from the simulation. Fourfold coordinated atoms are indicated by gray balls. Under/over-coordinated atoms are indicated as yellow (coordination 5), purple (coordination 3) and green (coordination 2) balls.

As for the first showcase application, we focused our activity primarily on the defect-induced crystal-to-amorphous transition in crystalline silicon. Such a phenomenon has attracted a huge number of experimental and theoretical investigations because of its fundamental interest from the point of view of the formation, nature and stability of amorphous state of matter as well as relevance to materials design and research problems. We have performed the first TBMD simulation of the response of a crystalline silicon (c-Si) lattice to random insertion of self-interstitials where large supercells (containing up to 276 atoms) were used.

The main goal was to provide a detailed characterization of both structural and electronic properties of irradiated samples and to show a comparison with amorphous silicon (a-Si) as obtained by direct quenching from the melt. Moreover, we have investigated the effects of a post-implantation thermal annealing on the topology and electronic structure of the amorphized material. The above simulation is intended as a first step towards an atomistic simulation of the ion-beam bombardment process. In Figure 1 we show how a crystal-to-amorphous transition is induced by increasing the absolute number of self-interstitial defects in the host lattice. There the particle-particle correlation function for three samples is reported. The number of inserted defects in sample a, b and c is 20, 30 and 60, respectively.

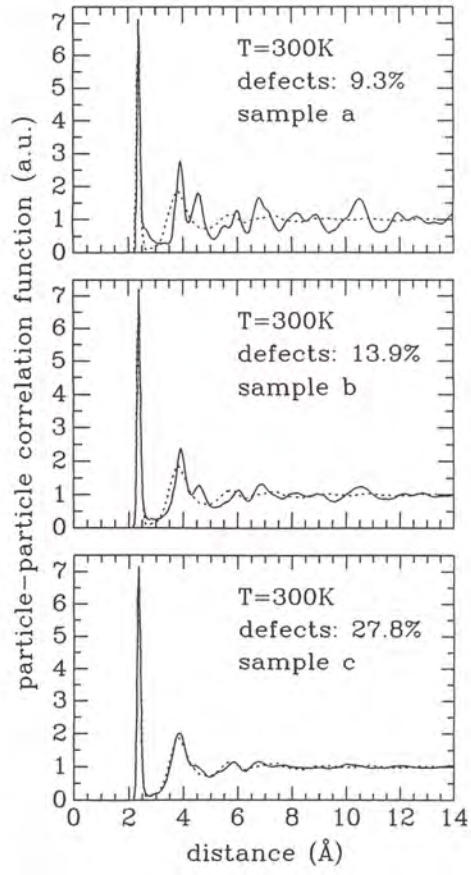

Figure 1. Pair correlation function of implanted silicon.

In Figure 1 we have also reported the particle-particle correlation function of a-Si as obtained by quenching a well-equilibrated 216-atom liquid silicon system. We observe that sample c (bottom panel) is pretty nicely disordered by the huge amount of defects and the crystal order is clearly lost at distances above the shell of second neighbours. The good agreement between the full-line and dotted curve indicates that the defect-induced amorphization process has created an amorphous network with structural properties similar to an overcooled liquid. In Plate 1 the a-Si structure resulting from the TBMD simulation is shown. An important part of the present research was the visualization and animation of TBMD results. This work was carried out in collaboration with P. Flükiger (CSCS) and A. Mangili (CSCS), respectively.

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Calculation contest between Boethius (using Arabic numerals) and Pythagoras (using an abacus), from "Margarita Philosophica" by G. Reisch, 1508.

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July–October 1994

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SSIP'94 Student project in collaboration with CSCS.
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Datcu, Mihai–Deutsche Forschungsanstalt für Luft- und Raumfahr (DLR) (Germany)
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PRDDO/M on the NEC SX-3: Applying Non-Empirical Quantum Mechanics to Extremely Large Molecules
May 1994

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SSIP participant: Program Structure Browser for the Annai Integrated Tool Environment
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La Cognata, Emanuele–Informatica, STS
Diploma work: Parallel and Distributed Generic Algorithms
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February 1993–continuing

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SSIP participant: PLUMP–Parallel Library for Unstructured Mesh Problems: Technical Specification
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Collaboration: Plasma Physics Project
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SSIP participant: Parallel Kernels for Krylov Subspace Methods
July–October 1994

Thomson, C.–University of Saint Andrews (U.K.)
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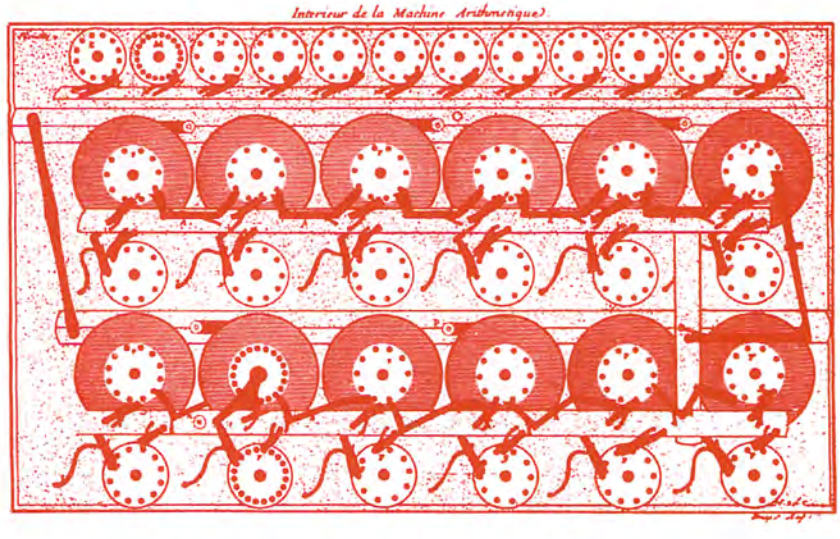
SSIP participant: Programming Environment for Parallel Iterative Solvers
July–November 1994

Verda, Paolo–Institut d'Informatique, Université de Fribourg
Diploma work: "Distributed Genetic Algorithms"
1994

Wu, Ling–Scientific Computing and Computational Mathematics, Stanford University (U.S.A.)
SSIP Participant: Parallelization of SOLIDIS
July–October 1994



The "Machine Arithmétique", an adding machine invented by B. Pascal in 1642.

COLLOQUIA

January 1994

Stricker, Thomas M.–School of Computer Science, Carnegie Mellon University (U.S.A.)
"Connections versus Messages."
Swiss High Performance Computing Seminar
CSCS; January 4, 1994.

Tomassini, Marco–CSCS
"Algoritmi genetici altamente paralleli per l'ottimizzazione matematica e combinatoria."
Seminar on Algoritmi Evolutivi
Milan (Italy); January 10, 1994.

Goedecker, Stefan–Cornell Theory Center, Cornell University (U.S.A.)
"Low Complexity Electronic Structure Calculations."
Swiss High Performance Computing Seminar
CSCS; January 13, 1994.

Stolcis, Luca–Centre for Advanced Studies, Research and Development in Sardinia (Italy)
"Computation of High-Reynolds Number Compressible Flows Using Unstructured Grids and Advanced Turbulence Models."
Swiss High Performance Computing Seminar
CSCS; January 14, 1994.

Scheidegger, Alfred–CSCS
"Forschungskooperationen in Japan."
ETH Zürich; January 18, 1994.

Schaer, Samuel–Centre de Recherches en Physique des Plasmas, EPFL
"Coaxial Plasma Gun in the High Density Regime and Injection into a Helical Field."
Swiss High Performance Computing Seminar
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February 1994

Hehre, Warren J.–Univ. of California and Wavefunction, Inc. (U.S.A.)
"Elucidation of Product Distributions in Organic Reactions."
Swiss High Performance Computing Seminar
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Scheidegger, Alfred–CSCS
"Strategic Resource Planning."
International Forum on Managing Computational Science for Industrial Competitiveness
Lugano; February 11, 1994.

Casavant, Thomas L.–Parallel Processing Laboratory, University of Iowa (U.S.A.)
"The Seamless Machine: A Latency-Tolerant RISC-Based Multiprocessor Architecture."
Swiss High Performance Computing Seminar
CSCS; February 18, 1994.

Decker, Karsten M.–CSCS
"Parallel Computing at the Swiss Scientific Computing Center (CSCS)."
University of Zurich; February 22, 1994.

Decker, Karsten M.–CSCS
"Parallel Computing at the Swiss Scientific Computing Center (CSCS)."
University of Neuchatel; February 25, 1994.

Müller, Andreas–CSCS
"High Performance Fortran (HPF)."
Swiss High Performance Computing Seminar
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Bern; March 17, 1994.

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"Effects of Ion-implantation in Silicon: A Computational Study."
General Meeting, Condensed Matter Division of the European Physical Society
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April 1994

Decker, Karsten M.–CSCS
"Design and Prototype Implementation of a Problem-solving Environment for Parallel Distributed Programming."
Fourth NEC-ETHZ Joint Workshop on Parallel Processing and Computational Science
NEC Corporation, Tokyo (Japan); April 12, 1994.

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"Parallel Computing at the Swiss Scientific Computing Center (CSCS)."
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"An Environment for Portable Distributed Memory Parallel Programming."
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May 1994

Decker, Karsten M.–CSCS
"Parallel Computing at the Swiss Scientific Computing Center (CSCS)."
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v. Hanxleden, Reinhard–Center for Research on Parallel Computation, Rice University (U.S.A.)
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Summer Term 1994.

June 1994

Scheidegger, Alfred–CSCS
"Managementaspekte eines projekt-orientierten Dienstleistungszentrums."
Swiss Bank Corporation
Zurich; June 16, 1994.

July 1994

Pohl, Bert–Seminar für Angewandte Mathematik (SAM), ETH Zürich
"Solving Large Systems of Odes: A Case Study."
Swiss High Performance Computing Seminar
CSCS; July 1, 1994.

Burrage, Kevin–Department of Mathematics, University of Queensland/Seminar für Agewandte Mathematik, ETH Zürich
"Deflation Techniques For Linear Systems Of Equations."
Swiss High Performance Computing Seminar
CSCS; July 4, 1994.

Rezny, Mike–Department of Mathematics, University of Queensland/Seminar für Agewandte Mathematik, ETH Zürich
"Client-server Models And Heterogeneous Computing."
Swiss High Performance Computing Seminar
CSCS; July 4, 1994.

Williams, Andrew–Department of Mathematics, University of Queensland/Seminar für Agewandte Mathematik, ETH Zürich
"The Implementation of a GCV Algorithm in a High Performance Computing Environment."
Swiss High Performance Computing Seminar
CSCS; July 4, 1994.

Cattaneo, Giampiero–Computer Science Department, University of Milan (Italy)
"Fluidodynamic of Percolation in Variable Geometry Environments."
CSCS; July 5, 1994.

Mauri, Giancarlo–Computer Science Department, University of Milan (Italy)
"Chaos and Cellular Automata."
CSCS; July 5, 1994.

Milani, Marziale–Physics Department, University of Milan (Italy)
"Radiation/Matter Simulation with Cellular Automata (semiconductor laser)."
CSCS; July 5, 1994.

Scheidegger, Alfred–CSCS
"Japan's Sprung vom Mittelalter in das 3. Jahrtausend."
Ingenieure für die Schweiz von morgen
Heerbrugg; July 5, 1994.

Hodoscek, Milan–Institute of Chemistry, Lubljana (Slovenia)
"Parallelisation of CHARMM for MIMD Machines."
Swiss High Performance Computing Seminar
CSCS; July 7, 1994.

August 1994

Rühl, Roland and William Sawyer–CSCS
"Tutorial on Parallel Computation."
Physics Computing (PC'94)
Lugano; August 22, 1994.

Decker, Karsten M.–CSCS
"The Joint CSCS-ETH/NEC Collaboration in Parallel Processing."
Physics Computing (PC'94)
Lugano; August 24, 1994.

Sawyer, William–CSCS
"Parallel Solution of Unstructured Mesh Problems."
IFIP WG 10.3, International Workshop and Summer School on Parallel Algorithms for Irregularly Structured Problems
Geneva; August 30, 1994.

September 1994

Decker, Karsten M.–CSCS
"Parallel Computing at the Swiss Scientific Computing Center (CSCS)."
Workshop Parallelrechner des Max-Planck-Instituts für Plasmaphysik (IPP)
Schloss Ringberg (Germany); September 9, 1994.

Gruber, Ralf–CSCS
"PE²AR Programmumgebung."
Workshop Parallelrechner des Max-Planck-Instituts für Plasmaphysik (IPP)
Schloss Ringberg (Germany); September 9, 1994.

Müller, Andreas–CSCS
"High Performance Fortran (HPF)."
Workshop Parallelrechner des Max-Planck-Instituts für Plasmaphysik (IPP)
Schloss Ringberg (Germany); September 9, 1994.

Travieso, Gonzalo–Physics Institute, University of Sao Paulo (Brazil)
"Molecular Dynamics on a Transputer Network."
Swiss High Performance Computing Seminar
CSCS; September 15, 1994.

Decker, Karsten M.–CSCS
"Parallel Computing at the Swiss Scientific Computing Center (CSCS)."
GMD, Inauguration of the C&C Laboratories
NEC Europe Ltd., St. Augustin (Germany); September 20, 1994.

Miller, Wolfram–Centre for Advanced Studies, Research and Development in Sardinia (Italy)
"Parallel Three-dimensional Lid-driven Cavity Flow on the IBM 9076-SP1 Scalable Parallel Computer."
Swiss High Performance Computing Seminar
CSCS; September 21, 1994.

Müller, Andreas–CSCS
"Architecture and Programmability of the NEC Cenju-3."
16th Speedup Workshop on Parallel and Vector Computing
Basel; September 22, 1994.

Moscato, Pablo–CeTAD, Universidad Nacional de La Plata (Argentina)
"Complex Systems for Complex Problems."
Swiss High Performance Computing Seminar
CSCS; September 28, 1994.

October 1994

Sehmi, Navtej–ABB Power Generation Ltd.
"A Solution for Kron's Eigenvalue Problem."
Swiss High Performance Computing Seminar
CSCS; October 12, 1994.

Dongarra, Jack–University of Tennessee and Oak Ridge National Laboratory (U.S.A.)
"Constructing Numerical Software Libraries for HPCC Environments."
Swiss High Performance Computing Seminar
CSCS; October 17, 1994.

Nonella, Marco–Physikalisch-Chemisches Institut, University of Zurich
"Application of Classical and Quantum Chemical Calculations to Photosynthetic Systems."
Swiss High Performance Computing Seminar
CSCS; October 20, 1994.

November 1994

Ramesh, Kalure Sridhara Murthy–Centre for Development of Advanced Computing, Pune University (India)
"Parallel Finite Element Solvers on PARAM."
Swiss High Performance Computing Seminar
CSCS; November 2, 1994.

Rahirkar, Kshama–Centre for Development of Advanced Computing, Pune University (India)
"New Algorithm for Matrix Transpose on a Distributed Memory Multiprocessor Network."
Swiss High Performance Computing Seminar
CSCS; November 3, 1994.

Sawley, Mark L.–Fluid Mechanics Laboratory, EPFL
"Parallel Computational Fluid Dynamics on the Cray T3D Using Different Programming Models."
Swiss High Performance Computing Seminar
CSCS; November 4, 1994.

Decker, Karsten M.–CSCS
"Towards Intelligent Programming Environments for Massively Parallel Systems."
International Symposium on Intellectual Facilitation of Creative Actions
Miel Parque Tokyo (Japan); November 15, 1994.

Decker, Karsten M.–CSCS
"The Future of Programming Environments for Massively Parallel Systems."
Third Symposium of the Utrecht University Center for Computational Science
Utrecht University (Netherlands); November 18, 1994.

Waser, Stefan–Center for Supercomputing Research and Development (CSRD) (U.S.A.)
"Finding New Parallelization Transformations Using Benchmark Programs."
Swiss High Performance Computing Seminar
CSCS; November 24, 1994.

Rühl, Roland–CSCS
"Extending High Performance Fortran for the Support of Unstructured Computations."
Journée sur la parallèlisation automatique et les supports run-time
EPF Lausanne; November 25, 1994.

December 1994

Martin, Olivier J.F–Institute for Field Theory and High Frequency Electronics, ETHZ
"A Numerical Green's Function Approach to the Computation of Electromagnetic Scattering by Arbitrary Media."
Swiss High Performance Computing Seminar
CSCS; December 14, 1994.

Sawyer, William–CSCS
"Application-Driven Development of an Integrated Tool Environment for Distributed Memory Parallel Processors."
First International Workshop on Parallel Processing
Bangalore (India); December 28, 1994.

COURSES AND CONFERENCES

International Forum on Managing Computational Science for Industrial Competitiveness

Paradiso-Lugano, February 10–11, 1994
Organized by CSCS
A two-day intensive seminar with case studies on how leading companies use computational science to increase their global competitiveness.

15th Speedup Workshop on Vector and Parallel Computing. Special Topic: Visualization and Networking

Cadro; March 17–18, 1994
Organized by the Speedup Society in conjunction with CSCS.

IFIP WG10.3 Working Conference on Programming Environments for Massively Parallel Distributed Systems

Monte Verità, Ascona; April 25–29, 1994
Organized by CSCS
Workshop, consisting of 40+ lectures, working groups, preprints and conference proceedings (published by Birkhäuser).

"Why Doesn't My Code Work on Your !@#$ Computer???"

ETH Zürich; June 8, 1994
Seminar organized by CSCS in collaboration with Les Hatton (Programming Research, Ltd.) on porting codes to CSCS computers.

6th Joint EPS-APS International Conference on Physics Computing

Palazzo dei Congressi, Lugano; August 22–26, 1994
Organized by CSCS in conjunction with the American Physical Society and the European Physical Society.
A week-long conference consisting of 80 lectures, working groups and conference proceedings (published by European Physical Society).

CSCS Summer Student Internship Program 1994 (SSIP'94)

CSCS; July 18–October 14, 1994
Organized by CSCS in collaboration with Luciano Colombo (University of Milan), Helmar Burkhardt (University of Basel), and Jan Korvink (ETHZ)
A two-week initial course in parallel computation followed by an eleven-week research project together with an advisor.

HPF Workshop

CSCS; October 18–21, 1994
Organized by CSCS in conjunction with Applied Parallel Research Inc.
Four-day course in High-Performance Fortran Programming.

PUBLICATIONS

Articles

Arnone, S., M. dell'Orto, A. Tettamanzi and **M. Tomassini.** "Highly Parallel Evolutionary Algorithms for Global Optimization, Symbolic Inference and Non-linear Regression". *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*, Lugano, Switzerland. Edited by **R. Gruber** and **M. Tomassini**. European Physical Society: 1994, 51–54.

Banfi, F. and **U. Meyer**. "An Environment for Maintaining AVS Modules." *Crosscuts* 3(1), 1994.

Beg, I., W. Ling, **A. Müller**, P. Przybyszewski, **R. Rühl** and **W. Sawyer**. "PLUMP: Parallel Library for Unstructured Mesh Problems." *Proceedings, IFIP WG 10.3 International Workshop and Summer School on Parallel Algorithms for Irregularly Structured Problems*, Geneva, Switzerland. Kluwer Academic Publishers: August 1994.

Bernardinelli, G., C.W. Jefford, **D. Maric**, C. Thomson and J. Weber. "Computational Studies of the Structures and Properties of Potential Antimalarial Compounds Based on the 1,2,4-Trioxane Ring Structure: I. Artemisinin-like Molecules." *Int. J. Quantum Chem. Biol. Symp.* 21 (1994): 117.

Chopard, B., M. Oussaidene, O. Pictet, R. Schirru and **M. Tomassini**. "Evolutionary Algorithms for Multimodal Optimization in Financial Applications." *Proceedings, Priority Programme Informatics Research, Massively Parallel Systems* Zurich: 1994, 139–142.

Clémençon, C., A. Endo, J. Fritscher, A. Müller, R. Rühl and **B.J.N. Wylie**. "An Environment for Portable Distributed Memory Parallel Programming." *Proceedings, IFIP WG10.3 Working Conference on Programming Environments for Massively Parallel Distributed Systems*, Monte Verità, Ascona, Switzerland (April 25–29, 1994). Edited by **K.M. Decker** and **R.M. Rehmann.** Basel, Switzerland: Birkhäuser Verlag, 1994, 159–170.

Clémençon, C, K.M. Decker, A. Endo, J. Fritscher, G. Jost, N. Masuda, A. Müller, R. Rühl, W. Sawyer, E. de Sturler, B.J.N. Wylie and **F. Zimmermann.** "Application-Driven Development of an Integrated Tool Environment for Distributed Memory Parallel Processors." *Proceedings, First International Workshop on Parallel Processing,* Bangalore, India (December 27–30, 1994). Edited by R. Rao and C.P. Ravikumar.

Clémençon, C., K.M. Decker, A. Endo, J. Fritscher, T. Maruyama, N. Masuda, A. Müller, R. Rühl, W. Sawyer, E. de Sturler, B.J.N. Wylie and **F. Zimmermann.** "Architecture and Programmability of the NEC Cenju-3." *SPEEDUP* 8(2), 1994.

Colombo, L. and **D. Maric** . "Defect-Induced Amorphization in Silicon." *Europhys. Lett.* (in press, 1994).

Cooper, W.A., **R. Gruber**, S. Merazzi, D.V. Anderson, and U. Schwenn. "Stability Calculations in MHD and Plasmas." *Proceedings, Biannual Conference on Computational Techniques and Applications* CTAC93 . Edited by D. Steward, H. Gardner and D. Singleton. World Scientific: 1994, 2–11.

De Sandre, G., L. Colombo and **D. Maric**. "Computer Simulation of Thermal Annealing Effects on Self-Implanted Silicon" *Mat. Res. Soc. Symp. Proc.* (in press 1994).

De Sturler, E. "IBLU Preconditioners for Massively Parallel Computers." In *Domain Decomposition Methods in Science and Engineering Proceedings, 7th International Conference on Domain Decomposition*, Pennsylvania, U.S.A. Edited by D.E. Keyes and J. Xu. American Mathematical Society: 1994.

De Sturler, E. and H.A. Van der Vorst. "Communication Cost Reduction for Krylov Methods on Parallel Computers." In *High-Performance Computing and Networking—Lecture Notes in Computer Science 797*. Edited by W. Gentzsch and U. Harms. Berlin: Springer-Verlag, 1994.

Decker, K.M. "Towards Intelligent Programming Environments for Massively Parallel Systems." *Proceedings, International Symposium on Intellectual Facilitation of Creative Activities*, Tokyo, Japan (November 14–15, 1994).

Decker, K.M. "Methods and Tools for Programming Massively Parallel Distributed Systems." *SPEEDUP* 7(2), 1994.

Decker, K.M., **J.J. Dvorak** and **R.M. Rehmann.** "A Knowledge-Based Scientific Parallel Programming Environment." *Proceedings, IFIP WG10.3 Working Conference on Programming Environments for Massively Parallel Distributed Systems*, Monte Verità, Ascona, Switzerland (April 25–29, 1994). Edited by **K.M. Decker** and **R.M. Rehmann**. Basel, Switzerland: Birkhäuser Verlag, 1994, 127–138.

Decker, K.M., **J.J. Dvorak,** and **R.M. Rehmann**. "User-driven Development of a Novel Programming Environment for Distributed Memory Parallel Processor Systems." *Proceedings, Priority Programme Informatics Research, Information Conference Module 3, Massively Parallel Systems*, Zurich, Switzerland, November 29–30, 1994: 40–47.

Decker, K.M. and **R. Rühl**. "SeRD—The Summer Internship Program." *Crosscuts* 3(1), 1994.

Decker, K.M. and **R. Rühl**. "The New NEC Cenju-3 System at CSCS." *Crosscuts* 3(3), 1994.

Decker, K.M. and **R.M. Rehmann**. *Programming Environments for Massively Parallel Distributed Systems*. Basel, Switzerland: Birkhäuser Verlag, 1994.

Dvorak, J. "A Programming Environment for Massively Parallel Programming." *Proceedings, Workshop on Artificial Intelligence for Object-Oriented Software Engineering, OOPSLA 1994* Portland, Oregon (1994).

Dvorak, J. "Integrating Different Paradigms in a Hybrid Computer Vision Tool." *Proceedings, Workshop on The Object Engine: Foundation for Next Generation Architectures, OOPSLA 1994* Portland, Oregon (1994).

Dvorak, J. "Two Perspectives on the EOOPS Theme." *Proceedings, Workshop on Embedded Object-Oriented Production Systems (EOOPS), OOPSLA 1994* Portland, Oregon (1994).

Dvorak, J. "Using *CLIPS* in the Domain of Knowledge-based Massively Parallel Programming." *Proceedings, CLIPS'94 Conference* Houston, Texas (September 1994).

Egli, W., O. Riccius, U. Kogelschatz, **R. Gruber** and S. Merazzi. "Computation of the Charge Density Distribution in a 3D Electric Field." *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*, Lugano, Switzerland. Edited by **R. Gruber** and **M. Tomassini**. European Physical Society: 1994, 535–542.

Estreicher, S.K., M.A. Roberson and **D. Maric**. "Hydrogen and Hydrogen Dimers in c-C, Si, Ge, and alpha-Sn." *Phys. Rev. B* 50 (1994): 17018.

Flükiger, P., E. Heeb, N. Masuda, **W. Sawyer**, C. Stern and F. Zimmermann. "Parallelization of Scientific Applications on Cenju-3." *Crosscuts* 3(3), 1994.

Flükiger, P.F., R. Gruber, A. Mangili and **D. Maric.** "Optimal User Support by PECCAM: Programming Environment for Computational Chemistry and Materials Science." *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*, Lugano, Switzerland. Edited by **R. Gruber** and **M. Tomassini.** European Physical Society: 1994, 573–578.

Gerteisen, E.A. "Massive Parallel Implementation of the Aircraft Euler Method and Performance Tests on Different Computational Platforms." *Crosscuts* 3(2), 1994.

Gruber, R. and **M. Tomassini** (Editors) *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*. Geneva: European Physical Society, 1994.

Hodous, M. "A Neighborhood, of Sorts." *Crosscuts* 3(2), 1994.

Maric, D. and L. Colombo. "Defect Induced Amorphization in Silicon: A Tight Binding Molecular Dynamics Simulation." *Mat. Res. Soc. Symp. Proc.* 316 (1994): 223.

Maric, D., M.A. Roberson and S.K. Estreicher. "Relative Stability of H^T vs. H^* and H_2^T vs. H_2^* in c-C, Si, Ge and *alpha*-Sn and Their Consequences." *Mat. Sci. Forum* 143–147 (1994): 1245.

Marynick, D.S., A. Derecskei-Kovacs, S.K. Estreicher, M.A. Roberson and **D. Maric**. "Toward Macromolecular Quantum Mechanics: the Optimization of PRDDO/M on the NEC SX-3." *Crosscuts* 3(2), 1994.

Meyer, U. "Human Capital & Mobility Program—Interactive Image Processing and Synthesis on Innovative Computer Architectures." *Crosscuts* 3(2), 1994.

Pommerell, C. and **R. Rühl.** "Migration of Vectorized Iterative Solvers to Distributed Memory Architectures." *Proceedings, Colorado Conference on Iterative Methods*, Breckenridge, Colorado (April 1994).

Pommerell, C. and **R. Rühl**. "Compiler Assisted Distributed Memory Parallelization of an Iterative Solver for Irregular Sparse Linear Systems." *Proceedings, Scalable High Performance Computing Conference*, Knoxville, Tennessee (May 1994).

Sawyer, W. "SSIP'94 to Repeat Previous Year's Success." *Crosscuts* 3(2), 1994.

Scheidegger, A. "Centri di supercalcolo per l'industria." *Pixel* 1(2) (1994): 11–13.

Scheidegger, A. "Co-operation Between Industry and Research Centres." *Supercomputer European Watch* (February 1994): 10–11.

Scheidegger, A. "Computational Science 'Goes' Industrial." *SPEEDUP* 8(1): 1994, 2.

Scheidegger, A. "European HPC Competitiveness Centres for Industry." *Proceedings, Lecture Notes in Computer Science—High-Performance Computing and Networking*. Number 797 Springer-Verlag: 1994, 103–108.

Scheidegger, A. "Instruments of Japan's Research and Development Policy." *Journal Wirtschaftskammer Schweiz-Japan* 1994 (4): 27–29.

Scheidegger, A. "Intensive Forschungs-kooperationen in Japan—Sicherung der internationalen Wettbewerbsfaehigkeit." *Neue Zürcher Zeitung*. April 12, 1994: 34.

Seidel, K. and **J-P. Therre**. "Remote Sensing Image Archive for National User Requirements." *Proceedings, European Data Networks and Earth Observation User Information Services: Survey and Consultation*. Rome, Italy (1994).

Stoll, E.P., A. Baratoff, **A. Mangili** and **D. Maric**. "Atom and Electron Motions on the Si(001) Surface Generated by First Principles Molecular Dynamics." *Helv. Phys. Acta* 67 (1994): 763–764.

Stoll, E.P., A. Baratoff, **A. Mangili** and **D. Maric**. "First-Principles Molecular Dynamics of the Si(001) Surface: Visualization of the Electron Density Dynamics by an Animation" *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*, Lugano, Switzerland. Edited by **R. Gruber** and **M. Tomassini**. European Physical Society: 1994, 33–36.

Stoll, E.P., A. Baratoff, **A. Mangili** and **D. Maric**. "Electron Dancing on the Si(001) Surface: A Video of First Principles Molecular Dynamics." *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*, Lugano, Switzerland. Edited by **R. Gruber** and **M. Tomassini.** European Physical Society: 1994, 33–36.

Suter, H.U., **D. Maric,** J. Weber and C. Thomson. "Quantum Chemistry and Drug Design." *Crosscuts* 3(3), 1994.

Suter, H.U., N. Paschedag, **D. Maric** and P.F. Meier. "The Hyperfine Structure of Muons in Silicon and Diamond Crystals." *Proceedings, First Electronic Computational Chemistry Conference* (1994).

Tomassini, M. "Massively Parallel Evolutionary Algorithms." *Journal of Modern Physics C* (to appear).

Tomassini, M. "Parallel Optimization through Cellular Evolutionary Algorithms." *Proceedings, ACRI Conference* (1994): 87–97.

Tran, T.M., D.R. Whaley, S. Merazzi and **R. Gruber**. "DAPHNE, a 2D Axisymmetric Electron Gun Simulation Code." *Proceedings, 6th Joint EPS-APS International Conference on Physics Computing*, Lugano, Switzerland. Edited by **R. Gruber** and **M. Tomassini**. European Physical Society: 1994, 491–494.

Technical Reports

Clémençon, C., K.M. Decker, A. Endo, J. Fritscher, G. Jost, N. Masuda, A. Müller, R. Rühl, W. Sawyer, E. de Sturler, and **B.J.N. Wylie**. *Application-Driven Development of an Integrated Tool Environment for Distributed Memory Parallel Processors.* CSCS-TR-94-01, April 1994.

Clémençon, C., J. Fritscher and **R. Rühl**. *Visualization, Execution Control and Replay of Massively Parallel Programs within Annai's Debugging Tool.* CSCS-TR-94-09, November 1994.

Gerteisen, E. *A Generic Data Structure for the Communication of Arbitrary Domain Splitted Mesh Topologies.* CSCS-TR-94-10, December 1994.

Gerteisen, E. *Implementation of Finite Volume Fluid Solvers into the PE²AR Database Environment.* CSCS-TR-94-11, December 1994.

Gruber, R. *PE²AR–Program Environments for Engineering Applications and Research.* CSCS-TR-94-06, August 10, 1994.

Müller, A. and **R. Rühl** *Extending High Performance Fortran for the Support of Unstructured Computations.* CSCS-TR-94-08, November 1994.

Nataf, F., F. Rogier and **E. De Sturler**. *Optimal Interface Conditions for Domain Decomposition Methods.* CMAP-301 (Centre de Mathématiques Appliquées, CNRS URA-756, Ecole Polytechnique France).

Rehmann, R. *Automatic Generation of Programs for a Scientific Parallel Programming Environment.* CSCS-TR-94-02, May 1994.

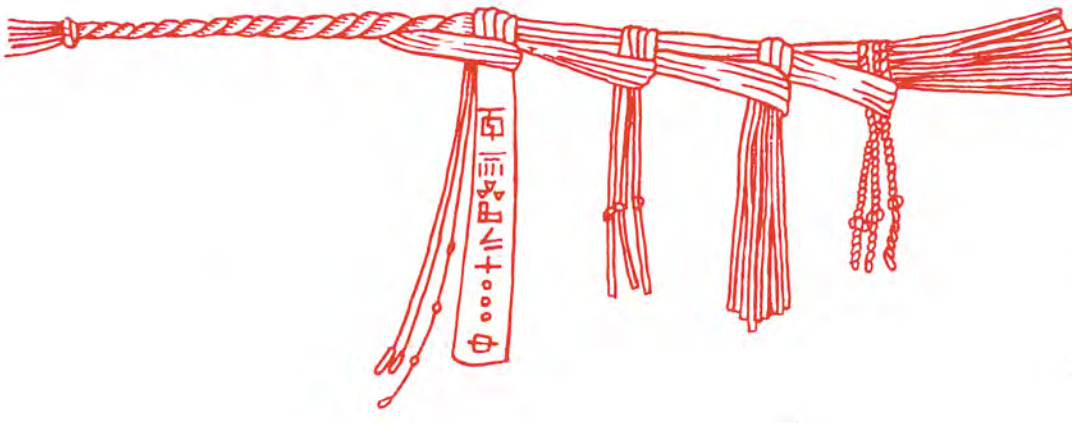
Sawyer, W., G. Kreiss, D. Sarenson and J. Lambess. *Arnoldi Method Applied to Burgers' Equation.* CSCS-TR-94-04, May 1994.

von Stürler, E. *Incomplete Block LU Preconditioners on Slightly Overlapping Subdomains for a Massively Parallel Computer.* CSCS-TR-94-03, May 1994.

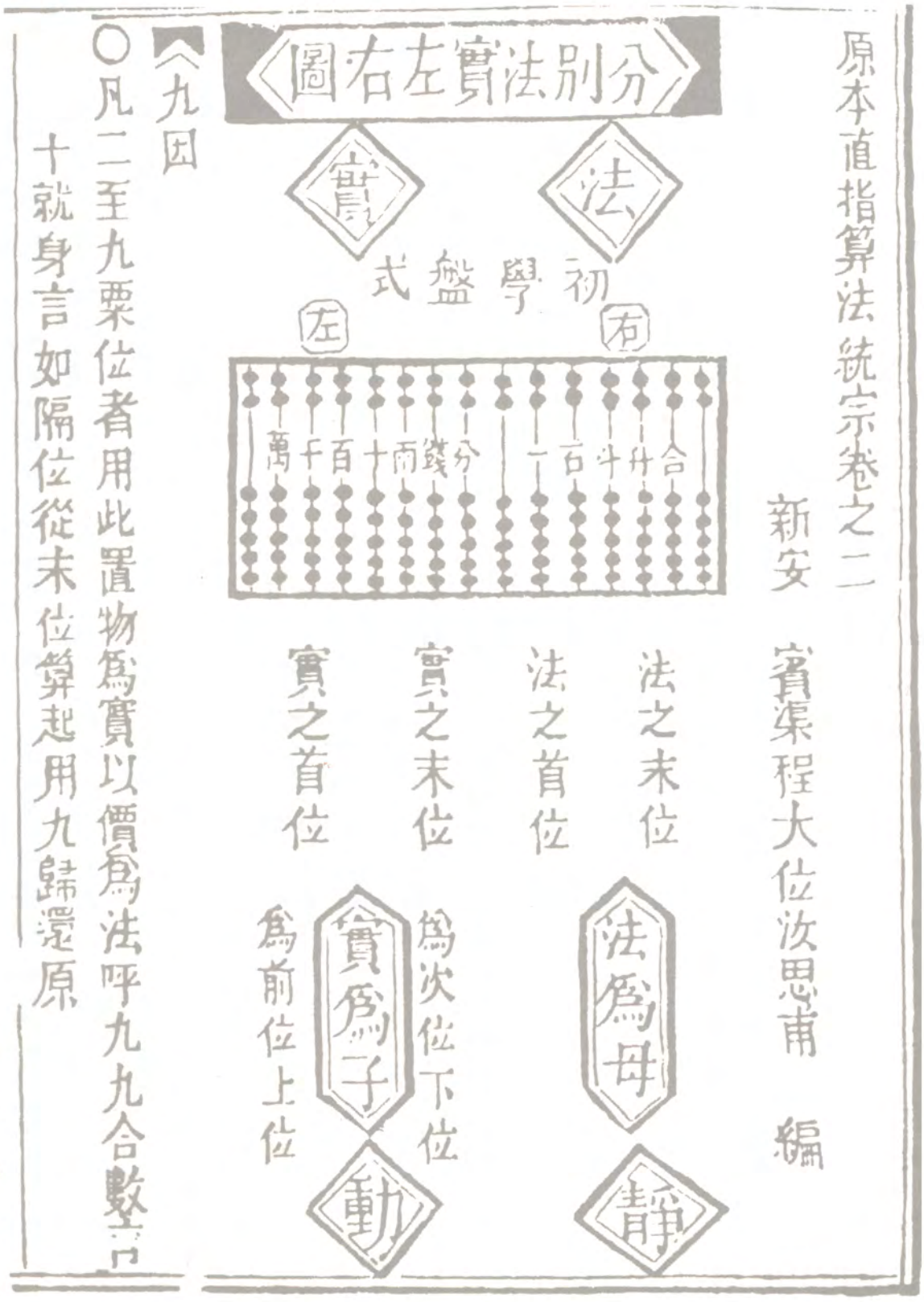
von Stürler, E. *A Performance Model for Krylov Subspace Methods on Mesh- based Parallel Computers.* CSCS-TR-94-05, May 1994.

Wylie, B.J.N and **A. Endo** *The Design and Realization of the "Annai" Integrated Parallel Programming Environment Performance Monitor and Analyzer.* CSCS-TR-94-07, August 1994.

Wylie, B.J.N., G. Cameron, M. White, M. Smith and D. McArthur. *PARAMICS: Parallel Microscopic Traffic Simulator.* EPCC-TR94-01, January 1994 (Edinburgh Parallel Computing Centre, Edinburgh, Scotland).



"Ketsujô" used for accounting in ancient Japan.



原本直指算法統宗卷之二

新安 賓渠程大位汝思甫 編

分別法實左右圖

法 實

初學盤式

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法之首位

實之末位

實之首位

法爲母 實爲子

爲次位下位

爲前位上位

靜 動

九因

○凡二至九乘位者用此置物爲實以價爲法呼九九合數

十就身言如隔位從末位算起用九歸還原

Chinese abacus: instructions, from "Suan fa tong zong", 1593.

ADDRESSES

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CSIA–Centro Scolastico Industrie Artistiche
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CRPP–Centre de Recherches en Physique des Plasmas (Research Center for Plasma Physics)
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IMAC–Institut de Mesure et Analyse des Contraintes (Institute for Stress Measurement and Analysis)
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IRRMA –Institut Romand de Recherche Numérique en Physique des Matériaux (Research Institute of Material Physics)
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SIC–Service Informatique Central (Scientific Computing Services)
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Olsen and Associates, Research Institute for Applied Economics
Seefeldstrasse 233, CH-8008 Zürich

Passera & Pedretti SA
via Adamini 10, CH-6900 Lugano

PSI–Paul Scherrer Institut
Badenerstrasse 569, CH-8048 Zürich

SMR SA
rue Dufour 109, CH-2500 Bienne

SNF–Schweizerischer Nationalfonds zur Förderung der wissenschaftlichen Forschung (Swiss National Science Foundation)
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Stream SA
Zona Industriale, CH-6825 Capolago

Ufficio del Lavoro (Employment Office), Dipartimento delle Finanze e dell'Economia
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CRIL Ingénierie, TERSUD-Bat. B
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106–112, bd. de l'Hôpital, F-75013 Paris

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F-93160 Noisy-le-Grand Cedex

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Heidenheimer-Strasse 5, D-71229 Leonberg

DLR–Deutsche Forschungsanstalt für Luft- und Raumfahr (German Aerospace Research Establishment)
D-82234 Wessling

Max-Plank Institut für Plasmaphysik
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Bolzmannstrasse, D-85748 Garching

MPI–Max-Planck Institut für Meteorologie
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LABEIN–Centro de Investigatión Tecnológica (Technological Research Center)
Cuesta de Olabeaga, 16, E-48013 Bilbao

RUSSIAN FEDERATION

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RAL–Rutherford Appleton Laboratory
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Inca "Quipamayoc" manipulating a "Quipo", with an abacus on his right. From a Peruvian Codex by Guaman Poma de Ayala, XVI Century.

ACRONYMS AND ABBREVIATIONS

ALWAN: A Language With A Name
ANNAI: one that leads or directs another's way (Japanese)
ATM: Ansynchronous Transfer Mode
AVS: Application Visualization System
BACS: Classification Scheme
BALI: Basel Algorithm Library
BLIPS: Basic Language for Iterative Parallel Solvers
BT: Block Tridiagonal
CFD: Computational Fluid Dynamics
CG: Conjugate Gradient
CLIO 3D: 3D ideal MHD equilibrium program
CSD: Crystal Size Distribution
CSR: Compressed Sparse Row
DMPAI: Data Modeling Programming Assistant Interface
DMPP: Distributed Memory Parallel Processors
EP: Embarrassingly Parallel
ESP: ElectroStatic Precipitator
EVA: Equipment for Voludensitometry Analysis
FDDI: Fiber Distributed Data Interface
FFT: Fast Fourier Transform
Gbyte: gigabyte, either 1000 megabytes or 1024 megabytes
GFLOPS: Giga Floating Point Operations Per Second
GUI: Graphical User Interface
HiPPI: High-Performance Parallel Interface
HPC: High-Performance Computing
HPF: High-Performance Fortran
IFS: Integrated Function Systems
IS: Integer Sort
ISDN: Integrated Services Digital Network
ISPE: Intelligent Skeleton Programming Environment
Kbit/s: Kilobit per second (1024 bit per second)
KSM: Krylov Subspace Methods
Mbit/s: megabit per second (1,048,576 bit per second)
Mbyte: megabyte, either 1 million or 1,048,576 bytes
MD: Molecular Dynamics
ME: Molecular Embedding
MFLOPS: Million Floating Point Operations Per Second
MG: MultiGrid
MHD: Magneto-Hydro Dynamics
MPI: Message-Passing Interface
MPP: Massively Parallel Processors
PDE: Program Development Environment
PE^{2}AR: Program Environment for Engineering Applications and Research
PECCAM: Programming Environment for Computational Chemistry and Materials Science
PLUMP: Parallel Library for Unstructured Mesh Problems
PMA: Performance Monitor and Analyzer
PRDDO/M: Partial Retention of Diatomic Differential Overlap/Modified
PRNG: Pseudo Random Number Generator (Library)
PST: Parallelization Support Tool
PVM: Parallel Virtual Machine
QUICKEST: Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms
RAID: Redundant Arrays of Inexpensive Disks
SESES: SEmiconductor SEnsor Simulation
SMPAI: Stencil Modeling Programming Assistant Interface
SOLIDIS: Simulation package for micro-actuators and sensors
SPARSKIT: SPARSe matrix computation KIT
SSIP: Summer Student Internship Program
TB: Tight-Binding
TBMD: Tight-Binding Molecular Dynamics
Tbyte: terabyte, 1,099,511,627,776 bytes (or 1 trillion bytes)
Tcl/Tk: Tool Command Language/Toolkit
TERPSICHORE: 3D ideal MHD stability program
UI: User Interface
ULTIMATE: Universal Limiter for Transient Interpolation Modelling of the Advective Transport Equations
VMC: Variational Monte-Carlo method

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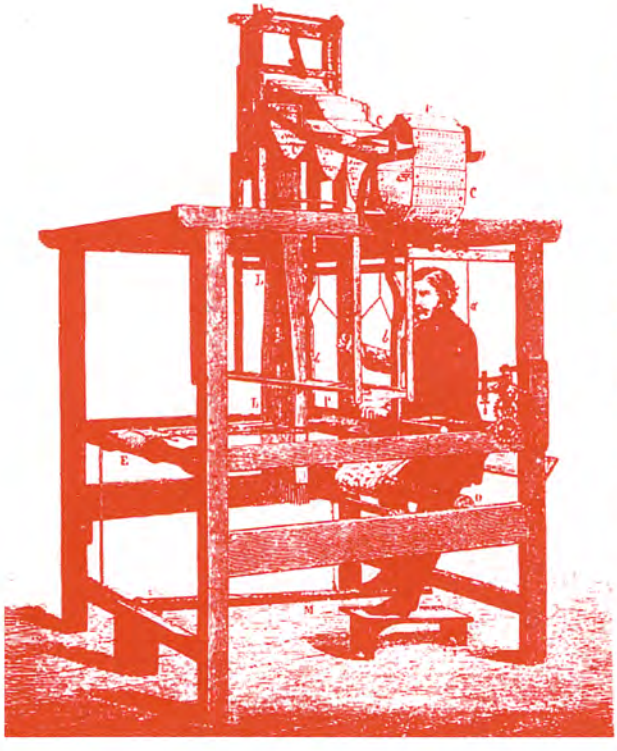

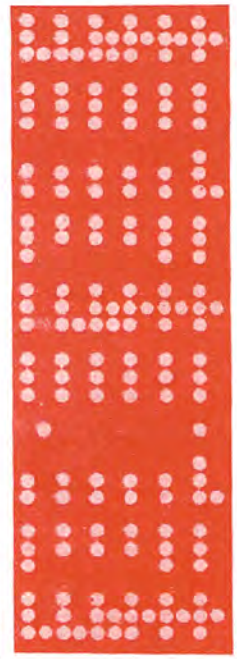

Punched card, invented by J-M. Jaquard to "program" weaving-looms.

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