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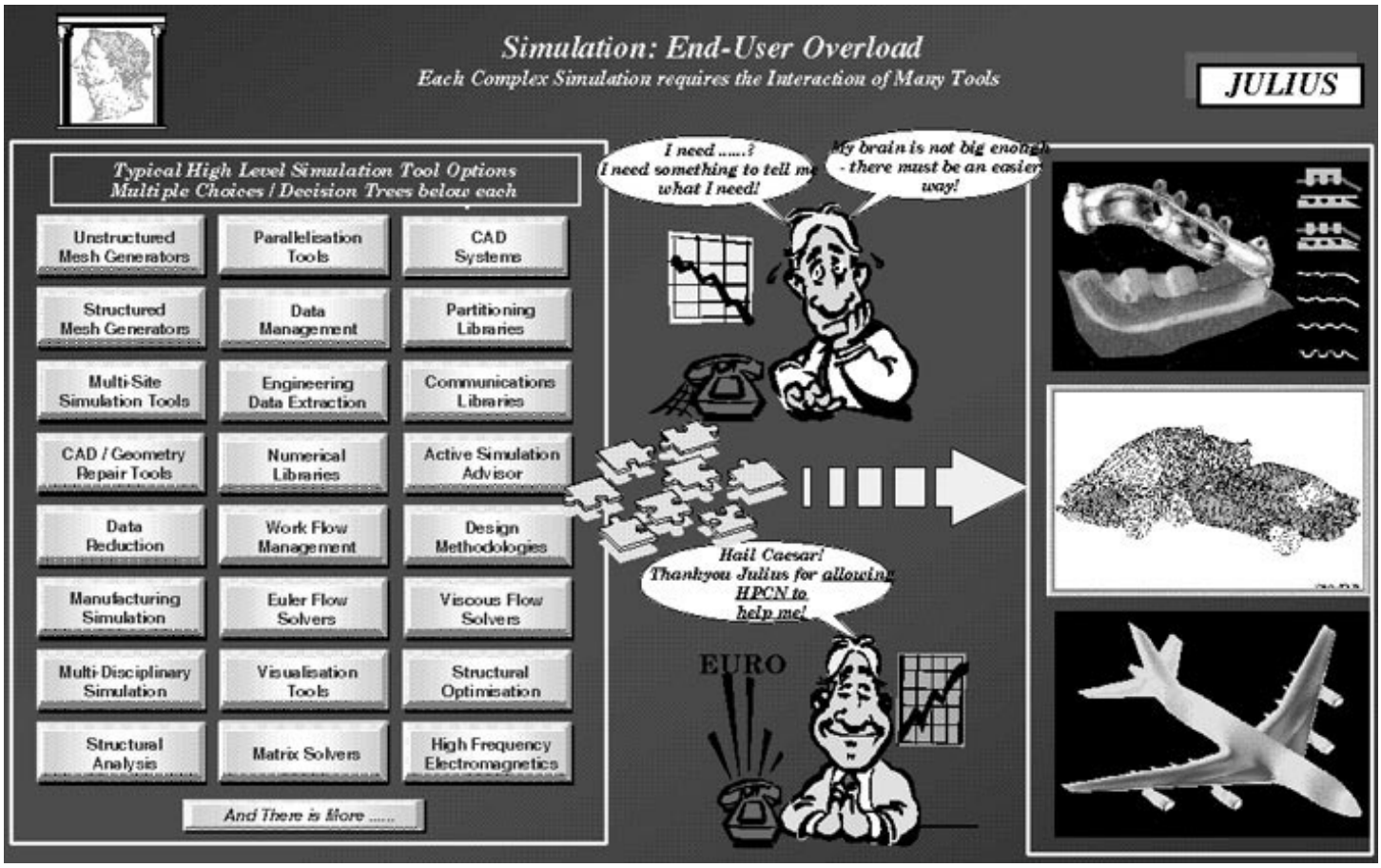

End-user engineer overload. See article page 20.

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Editorial

Dear readers

To many of our users it must have been quite a shock when they heard about it.

At the end of August, Jean-Pierre Therre, who led CSCS since 1996 with great idealism and success, decided to step down as director. He felt he had not enough support from part of the staff at Manno to continue his work. I would like to thank Jean-Pierre for all he has done for CSCS in the last three years. Without him CSCS would not be in such a good shape as today.

Like many other academic institutions these days, CSCS must adjust to the decreasing available funds. Not everything that has been possible in the past will be possible in the future. Priorities will have to be selected, new ways of financing must be found. It is not surprising that discussions of this kind cause intensive reactions sometimes.

In spite of the current difficulties of financing large investments in the hardware, I am convinced CSCS in Manno has a promising future. The current reorganisation process aims at anchoring CSCS more firmly in Ticino. We are searching close relations with nearby institutions. The core mission of CSCS—offering high-end supercomputing power to Swiss research—will remain as it is. In addition, the exchange with universities and industry shall be strengthened even more. At the moment several groups are working on redefining of the future products and the future structure of CSCS.

In the next issue of CROSSCUTS I will be able to tell you more about how CSCS will look in future. CSCS has proven in the past that excellent work can be done in Manno.

I feel sure, that excellency must and will remain the highest priority at CSCS.

Hans-Peter Wessels, Director ad interim

Contact

Hans Peter Wessels (wessels@cscs.ch) ■

Publishing Editor: H.-P. Wessels
Managing Editor: C. Moor
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PROGRAMMING ENVIRONMENT SUPPORT GROUP (PES-SSU)

Angelo Mangili and Djordje Maric (CSCS/SCSC)

With the recent reinforcement of the Programming Environment Support (PES) group, we would like to draw the attention of CSCS/SCSC users to this important resource of competence. The support and service offered by this group is responsible for the optimal and user-friendly usage of the HPC power installed in Manno.

Since the beginning of CSCS/SCSC, the Programming Environment Support Group (previously called the Optimization Group) has been an important user support oriented group. The group provides high quality support and competencies to users for languages, compilers, development tools, analyzers and programming paradigms, "above" the OS level as well as "below" the level of mathematical, scientific and engineering libraries.

1. Programming Environment Support Group Goals

The group goals are to:

- provide to all users programming environment support and related solutions for an efficient and user-friendly access to CSCS/CSCS computing resources, and
- increase the usage efficiency of the installed power through interaction and cooperation with the members of other CSCS/SCSC groups. In particular, provide the Production Systems Group (PSG) with feedback on the production environment and collaborate with the Advanced Numerical Algorithms group (ANA), the Scientific Visualization group (SciVis), Application Support (engineering, chemistry, …) in order to optimize the benefits of a multidisciplinary approach and knowledge transfer.

The newly restructured group is intended to reinforce and streamline the support activities of the CSCS/SCSC production systems. The benefits of such a support activity has been demonstrated in several occasions. Mainly by the impressive and world-wide recognized results of the NEC-CSCS Task Force project, the real-time follow-up on user problems, performance monitoring and optimization, and the operational distant learning environment for user education and user information.

The group is composed of:

Dipl. Ing. Info. EPFL Angelo Mangili: Head, Programming Environment Support Group

Dipl. Ing. Info. ETHZ Mauro Ballabio: Senior application analyst, member of the SX-4 Task Force

Dr. Laurent Gasser: Application analyst, member of the SX-4 Task Force

Dr. Michael Hodous: Senior application analyst, PES Help Desk

Dr. Manfred Thüring: Application analyst, Exemplar parallelization support

2. Programming Environment Support Group Duties

Helping users to port and tune their code has two main benefits: the user realizes improved code efficiency and CSCS/SCSC is guaranteed better efficiency, usage and workload of its production systems. Moreover, the help desk organization follows up on user problems in such a way that users are able to shorten program development time and production turn-around and reach a solution state faster.

2.1 Programming Environment Support Help Desk

Through the help desk, the group can:

- ensure prompt and efficient support to reported user problems,
- consult with other colleagues at CSCS/SCSC to resolve user problems,
- fix bugs in user codes,
- processing (pre/post) of user data, and
- give technical assistance for image and video generation.

2.2 User Code Support

The code support activities offered to users include:

- helping in development/re-engineering,
- porting/tuning,
- optimizing,
- vectorizing/parallelizing,

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NEWS FROM THE SERVICES SECTION

E450—New File Server

As previously announced, all user services are now accessible through dom.cscs.ch. Dom is a SUN Enterprise 450 equipped with 2 processors, 1 GB memory and 90 GB disks. Information can be found on

http://www-users.cscs.ch/ all/sun/index.html

Problems should continue to be addressed via e-mail to

help@cscs.ch ■

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- supporting programming environments (compiling, debugging, analysis),
- processing (pre/post) and converting of data and GUI's,
- aiding in efficient usage of available libraries,
- increasing portability of code and data files across multiple platforms,
- promoting programming language standards,
- supporting the most common languages: F77, F90, HPF, C/C++ and
- supporting the most common programming paradigm: MPI, PVM.

2.3 User Consultancy

The group's consultancy activities help users find the most appropriate platform for their work ensures that users

- get the most benefit from their code and
- make optimized usage of CSCS/SCSC installed power (today and in future).

2.4 User Education

The group organizes programming environment-related courses and seminars as part of the overall CSCS/SCSC educational program.

In particular, the group attempts to direct users towards new programming paradigms and architectures, and standards for portability and correctness

2.5 User Information

The group is charged with writing and maintaining printed and online technical documentation (such as the CSCS/SCSC User Guide) and implementing modern information and communication solutions to disseminate information to a wide audience in a cost-effective way.

2.6 User Projects

The group can assist in user projects through code porting, optimizing (vectorization and parallelization), tuning and validation, as well as supporting project-related student stages in Manno.

3. General Strategies of the Group

The group achieves its goals through several strategic approaches:

- being pro-active: maintaining good contacts with users but also making an effort to attract new users. This task should be based on permanent monitoring and analysis of systems usage and performance, further leveraging the Performance Monitoring Tool developed by M.Ballabio. Selecting the most appropriate projects that really need help and focus human resources accordingly.
- promoting horizontal synergies: Interacting and cooperating with the members of other CSCS/SCSC groups, in particular: Production Systems (PSG), Advanced Numerical Algorithms, Scientific Visualization (SciVis), Application Support (Engineering, Chemistry, …) in order to optimize the benefits of a multidisciplinary approach and knowledge transfer.
- promoting user contacts: Interacting with the users to understand and anticipate their needs, and when appropriate, promoting tele-working technology to improve daily interaction.
- evaluating emerging technologies: Permanent development of competencies/excellence in core technologies. Evaluation and benchmark of new HW/SW technology to maintain leading edge competencies and expertise for CSCS/SCSC long-term plans, budget planification and to improve user support.

For additional info and/or a support request please contact help@cscs.ch.

Contacts
Angelo Mangili (amangili@cscs.ch)
Djordje Maric (dmaric@cscs.ch)

GETTING TO KNOW TWO NEW COLLABORATORS AT CSCS/SCSC

Claudia Moor (CSCS/SCSC)

At the beginning of 1998, two new collaborators joined the CSCS/SCSC user services section: Marco Consoli and Manfred Thüring. Both will be in direct contact with the center's users and contribute to maintaining the user support services at a high level.

The following two profiles introduce Marco and Manfred to CROSSCUTS readers and, in particular, to the users of the CSCS/SCSC compute facilities.

Marco and Manfred are eager to know you too and to further improve the communication between the center and its user community: so don't hesitate to contact them directly!

Marco Consoli took over the User Support Interface function at the beginning of 1998. His voice might already be known to some CSCS/SCSC users, since Marco is responsible for the Help Desk.

Marco was working in electrical engineering when his growing interest in communication technologies and computer science pushed him to a formal education in this field. In 1997 he received a diploma in computer science, granted by the local University of Applied Sciences (STS/SUPSI) in Manno.

Marco—who adores reading about scientific visualization, artificial intelligence and astronomy—is currently busy familiarizing himself with all the users and their scientific projects at CSCS/SCSC. Marco uses email and postal mailings as well as direct telephone contact to communicate with users but puts special emphasis on the importance of the web and online documentation for information distribution.

After the first months of working at CSCS/SCSC, Marco is enthusiastic and is optimistic about his future work at the center. You can reach Marco at mconsoli@cscs.ch, help@cscs.ch or 41 91 610 82 10.

Monthly Systems Maintenance

Hardware and software maintenance of all production systems takes place every first Monday of the month. Hardware preventive maintenance is a fixed time (4 hours) from 8am until noon, with possible dedicated time for benchmarking from noon until 2pm, and finally software maintenance (variable time) in the afternoon. After shutdown and reboot the systems are opened again to the users. ■

Manfred Thüring joint the SSU Section in the spring of 1998 as an Application analyst. He graduated from the University of Bern in1997 with a Ph.D. in Earth Sciences. During that time Manfred spent one year at the Johns Hopkins University in Maryland USA and then went back to the University of Bern as a postdoc.

Manfred's work experience includes project work at the Informatikdienste of the University of Bern as well as in the private sector in the field of geotechnical engineering. Manfred is a very communicative person and his goals are ambitious; he says that he doesn't want his work for the user support section to be only "screen-oriented." One of his goals is to further improve the working/programming environment of the center's HP Exemplar facility according to the users' needs and requirements. In his opinion "science as such is hard enough" and a computing center should therefore help researchers in finding solutions. He also would welcome an upgrade of the HP Exemplar facility.

Like his colleague Marco Consoli, Manfred insists on the importance of the Internet as a communication channel to make CSCS/SCSC known to the whole Swiss and international academic community.

And what about life in Ticino? Manfred adores the vicinity of the lakes, the mountains and nearby Italy. And—he doesn't mind being addressed in Swiss-German when shopping in Lugano… You can reach Manfred at thuering@cscs.ch or 41 91 610 82 33.

Let's wish to both, Marco and Manfred, all the best for their future work at CSCS/SCSC!

Contact
Claudia Moor (haeberli@cscs.ch) ■

The SX-4 Task Force Projects (Part 2)

Djordje Maric (CSCS/SCSC), René Hausammann and Charles Henriet (NEC European Supercomputer Systems, Manno)

Numerical Simulation of Transition and Turbulence: IFD Project–Optimization of Computer Codes for Numerical Simulation of Transitional and Turbulent Fluid Flows

L. Kleiser, N. A. Adams, C. Mielke, T. Wintergerste (Institute of Fluid Dynamics, ETH Zurich) and M. Ballabio (CSCS/SCSC)

1. The Scientific Objective

Fluid flow is of importance in numerous technical devices and in almost any practical applications it is at least partially turbulent. For design problems involving fluid flow, computational fluid dynamics (CFD) has become an indispensible tool and is used increasingly for subtle optimization tasks. Since it is impossible to resolve all scales of a turbulent flow with practical relevance, CFD requires appropriate turbulence models. A related unsolved problem of CFD is the prediction of laminar-turbulent transition.

Present turbulence models suffer significantly from shortcomings in knowledge about the behavior of transitional and turbulent flows and from the lack of reliable reference data. The

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scientific part of this project addresses the direct numerical simulation (DNS) of incompressible and compressible transitional and turbulent boundary-layer flows. Within the DNS approach, all relevant flow scales are resolved and no modeling is required. A major part of the project is the DNS of the turbulent supersonic boundary layer along a compression ramp, which is unprecedented in terms of physical complexity and is currently one of the most ambitious DNS projects worldwide.

2. The Time to Solution

The computational effort of a DNS, even for simple configurations, is so large that it can only be achieved by using the most powerful state-of-the-art computers. Even then it requires the use of highly optimized computer codes.

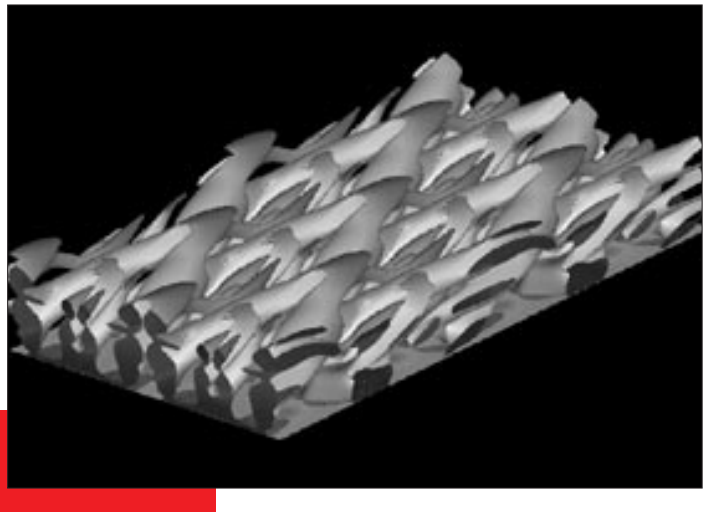

Figure 1: *Visualization of vortical structures generated during laminar-turbulent transition in supersonic flow.*

A few hundred CPU hours are required on an SX-4 for the simulation of "laminar-turbulent transition." For the direct simulation of "turbulence" one has to compute the evolution of the turbulent flow in time over several hundred to thousand samples to obtain reliable statistics. The computing time is on the order of several thousand CPU hours for the DNS of turbulent compression ramp flow.

3. The Task Force's Achievements

Written in FORTRAN 77, the program COBOLT_S used for the compression ramp simulation contains 19,000 lines of code with more than 800 routines. It has been serially optimized and a complete parallelization has been realized by using automatic and hand-tuned parallelization.

4. The Outstanding Result

Today, the Task Force has accomplished a significant optimization of the COBOLT_S program: starting from an optimized serial version running at 1.1 GFLOPS, the team has reached 8.3 GFLOPS with a speed-up factor of 7.5 on 8 processors. Similar speed-up has been obtained for other simulation programs used for transition research, with up to 12.6 GFLOPS on 8 processors.

Performance as a function of CPUs demonstrates the excellent speed-up behavior of COBOLT_S:

# CPU	GFLOPS	Speed-up
1	1.1	1.0
2	2.2	2.0
4	4.2	3.8
8	8.3	7.5

The memory requirements are typically large for this type of direct numerical simulation and can reach up to 4 Gbytes.

5. The Added Value to Research

The research at ETH/IFD on transitional and turbulent flows (complementary to and along with the efforts at EPFL/IMHEF), places Switzerland among the leading countries in this area.

With thousands of CPU hours needed for the time to solution, CPU time is most critical. Therefore, there is a strong interest in making optimum use of the available computing resources. The computer codes developed at IFD and optimized by the Task Force perform extraordinarily well on the SX-4 architecture.

Contacts
Djordje Maric (dmaric@cscs.ch)
René Hausammann (rhausammann@nec.ch)
Charles Henriet (chenriet@cscs.ch)
Leonhard Kleiser (kleiser@ifd.mavt.ethz.ch)
Niklaus A. Adams (adams@ifd.mavt.ethz.ch)
Christian Mielke (mielke@ifd.mavt.ethz.ch)
Torsten Wintergerste (torsten@ifd.mavt.ethz.ch) ■

RECENTLY INSTALLED SOFTWARE

Dom: fgen v0.3 available
Dom: nedit v5.0.2 available
Dom: ImageMagik v3.8.8 with extension for HDF, JPEG, MPEG, TIFF formats available
Dom: GNU software available: gcc 2.8.1, gzip 1.2.4, gmake 3.76.1 and gtar 1.12
Dom: psutils available
Dom: xemacs v20.3 available
Dom: xv v3.10a available
Dom: perl v5.004 available ■

Chemistry Software at CSCS/SCSC: Update

Stefan Portmann (CSCS/SCSC)

What software is currently installed?

Table 1 shows the chemistry software currently available. More detailed information for each application is listed on the corresponding web page (http://www.cscs.ch/Official/Services/AppSoft_ListCCM.html). The user is strongly encouraged to consult this page, since it provides links to on-line manuals and homepages of the applications, job submission scripts and other useful information. Program updates are posted there as well as detected bugs. The page also lists what application can be found on a given platform (Table 2). It covers most of the frequently asked questions and should be the first entry point for both new and experienced users to get information about chemistry software installed at CSCS/SCSC.

Ab Initio / Density Functional Methods:	
ADF	Density functional program
Amoss	Hartree-Fock based electronic structure calculations
Castep	A plane wave density functional program for solid state and surface calculations
Gamess-US	Package for Hartree-Fock and semi-empirical methods
Gaussian94	General computational chemistry package for Hartree-Fock, CI and DFT methods
Meldf-x	Single-/multi-reference CI
Molcas-4	Multiconfiguration SCF and CI, MCSCF, CASSCF
Molpro	Multiconfiguration SCF and CI, MCSCF, DFT
Molfdir	Relativistic Dirac-Fock-CI
Prddo/M	Approximative Hartree-Fock for very large molecules
TURBOMOLE	Program package for ab initio electronic structure calculations.

Semiempirical Methods:	
Mopac6	
Mopac7	A semiempirical molecular orbital package

Molecular Dynamics:	
AMBER	Assisted model building with energy refinement
CHARMM	Molecular mechanics, MD
Moil	Molecular dynamics
Moldy	General-purpose molecular dynamics simulation program
TBMD	Tight-binding molecular dynamics

Table 1: Installed chemistry application software at CSCS/SCSC

Program	SX-4 gottardo.cscs.ch	SPP castor.cscs.ch	HP hp[1..8].cscs.ch
ADF		•	•
AMBER	•		•
Amoss	•		
Castep		•	•
CHARMM		•	•
GAMESS-US		•	•
Gaussian94	•	•	•
Meldf-x		•	•
Molcas-4		•	•
Molpro	•	•	•
Moil		•	•
Molfdir		•	•
Mopac7		•	•
Moldy		•	•
PRDDO	•	•	•
TBMD	•		•
TURBOMOLE		•	•

Table 2: Platform Availability of the software packages at CSCS/SCSC

Contact
Stefan Portmann (portmann@cscs.ch) ■

User Support for Engineering: A Status Report

Vaibhav R. Deshpande and Karsten M. Decker (CSCS/SCSC)

1. Introduction

Last year, responding to user requirements for increased availability of engineering-related application software on its high-performance computing environment, CSCS/SCSC expanded its computational fluid dynamics (CFD) and related preprocessing application portfolio and reinforced user support in this area [1]. The application packages FLUENT (comprising FLUENT, FLUENT/UNS and RAMPANT), CFX (comprising CFX-Build, CFX-Solver and CFX-Visualize) and the preprocessor tool ICEMCFD were made available on the CSCS/SCSC computing platforms. This enriched portfolio of application software provided a foundation for the solution of a wide variety of flow problems.

To help exploit this software, CSCS/SCSC's *Interdisciplinary and Industrial Applications Group* (I^2A) provided support and expertise to both the industrial and academic user communities. This article briefly highlights the different dimensions of the support and services which the I^2A group has directly or indirectly extended to its users in the past year.

2. Scope of the Support Activities

2.1 Help Desk

After successful installation and testing of the packages on the different computing platforms (in cooperation with CSCS/SCSC's services section SSU), the software was made available to the user community.

Information about the access and use of software was distributed through CSCS/SCSC's Internet site. Personal queries from ETH Zurich, EPF Lausanne, PSI and Swiss cantonal universities were and continue to be handled on an individual basis.

2.2 Evaluation and Benchmarking

Based on a request from the ABB Corporate Research Center in Baden-Dättwil, CSCS/SCSC carried through the application-specific performance evaluation of the CFD software RAMPANT on the multiprocessor NEC SX-4 system by running a large test case of practical importance for ABB. Similarly, a project for Sulzer was undertaken to qualify the sustained performance of the finite element package ABAQUS on the computing platforms at CSCS/SCSC for solving one of Sulzer's large structural analysis cases.

Significant amounts of computer and human resources were invested in both of these evaluations, clearly demonstrating CSCS/SCSC's dedication to provide user-driven services not only to the academic sector, but also to industrial segment.

2.3 Education and Information Exchange

Similar to last year, support was provided also to the educational initiatives of CSCS/SCSC. Using the available on site software and support, students of the *Computer and Communications Camp* (C^3) [2] were intensively trained and closely supervised during their two-week projects.

The *One-day Workshop on Industrial Multi-Phase Flow Modeling* was organized by CSCS/SCSC on November 14th, 1997 at ETH Zürich in cooperation with ERCOFTAC's Leonhard Euler Competence Center for CFD. At this workshop, people from industry, academia and research enhanced their understanding of multi-phase flow modeling. One of the highlights of this workshop was the active involvement of industrial companies such as Lonza SA, Novartis SA, Sulzer and ABB.

Furthermore, the *23rd SPEEDUP Workshop on Process Engineering* was successfully conducted by CSCS/SCSC in cooperation with the Leonhard Euler Research Center on March 19th and 20th, 1998 at ETH Zurich. Here again, the active participation of the industrial frontrunners such as ABB, British Aerospace, Daimler Benz, Novartis, Rieter, and Sulzer Innotec gave an opportunity to know more about industrial needs and share their practicalities with regard to process engineering.

2.4 Modeling

Using the CFD application packages, it is possible to address a wide variety of flow problems. However, modeling of a physical phenomenon using these packages still requires considerable expertise and knowledge with regard to fluid dynamics—heat transfer on one hand and computational techniques on the other. The focus of the overall support activity was, therefore, on providing expertise to those without the adequate experience and/or resources to pursue their own modeling.

For instance, a feasibility study was done for development of a radiation model for the solar thermochemical reactor [3], as part of a project support to the Australian National University in collaboration with Australian, German, Malaysian, and Swiss industrial partners (financially supported by the Swiss Office of Energy).

A recent project from Earth Sciences Institute in Cadenazzo (Istituto di Scienze della Terra), part of the Scuola Universitaria Professionale della Svizzera Italiana (SUPSI), to model the free-surface flow of a mountain river to evaluate the hydraulic dangers is another example. Apart from the preparation of the complicated topological features of the geography from the point of discretizing the domain for flow simulation, this work involves the development of a computational model for simulation of the flow through the basin.

Keeping in mind these and other complex physical simulation needs of the user community, evaluation and extension of the modeling capabilities of the packages, specially for multi-phase flow modeling was seen as crucial. This is specially the case, since the strong non-linearities and complexities of multi-phase flows often makes the black box treatment of the available software grossly inadequate. Hence, as part of an ongoing international collaboration with the National Chemical Laboratory (NCL), in India, we have been developing a basic framework of mathematical models for industrial flow simulation. Gas-liquid flows in stirred tank reactors [4] and in bubble columns are being investigated for application in pharmaceutical, chemical and other process industries. The knowledge and expertise gained has proved valuable for tackling other diverse flow problems.

2.5 Intergroup Synergies

Post-processing of the numerical data obtained from the solvers is critical to the CFD user community to enhance the understanding of the underlying physics. Collaboration with the experts of CSCS/SCSC's Visualization Group ensured that the data obtained from the aforementioned packages could be post-processed using state-of-the-art techniques [5].

Another example of fruitful cooperation for the benefit of user community is the joining of forces with the Software Technology Cluster within I²A. They have developed a prototype of the *General Resource and Application Management Environment* (GRAME) in collaboration with Sun Microsystems [6] to ease the access and usage of distributed computing resources for the users. Using two different packages (the commercial CFD package FLUENT and the in-house CFD software SPARE, developed at NCL), an application simulating the flow in bubble column reactor was set-up to investigate its capabilities.

Advanced selection of remote compute servers, monitoring of job status and pre-defined application parameters was demonstrated while either FLUENT or SPARE was executing on a remote host. Uniformity of the user interaction and data representation, irrespective of the running application proved the usefulness of the project.

3. Outlook

With the advancement of CFD as a whole, the user community will continue to benefit from the availability of software and support on the powerful HPC environment at CSCS/SCSC. Cutting edge modeling techniques in CFD coupled with state-of-the-art visualization tools will make it possible for the users to better understand the complex physical processes contributing to their overall progress. In the future, we look forward to consolidating and extending our support not only in CFD but in computational structural mechanics for the benefit of the user community. The recent availability of the PAM suite of software on the CSCS/SCSC computing environment can be seen as a step in this direction.

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Contacts
Vaibhav R. Deshpande (vaibhav@cscs.ch)
Karsten M. Decker (decker@cscs.ch) ■

C³ Computing and Communications Camp 1998

Bernardo Zumthor (CSCS/SCSC)

For the fourth consecutive year, CSCS/SCSC organized the C³ Computing and Communications Camp in Manno. The summer camp, sponsored by the Canton of Ticino within the education initiative called "Ticino Campus", focussed on scientific computing (computer simulation). The camp is designed for upper level high school students who are particularly interested in scientific simulation applications: they come from all parts of Switzerland and from the "Regio insubrica", the neighboring Italian region that includes the provinces of Como, Varese and VCO (Verbano-Cusio-Ossola).

This article gives an overview of the camp organization and activities. More information can be found on the corresponding Web pages ("www.cscs.ch/C3") showing a variety of projects developed by the students together with advisors and assistants.

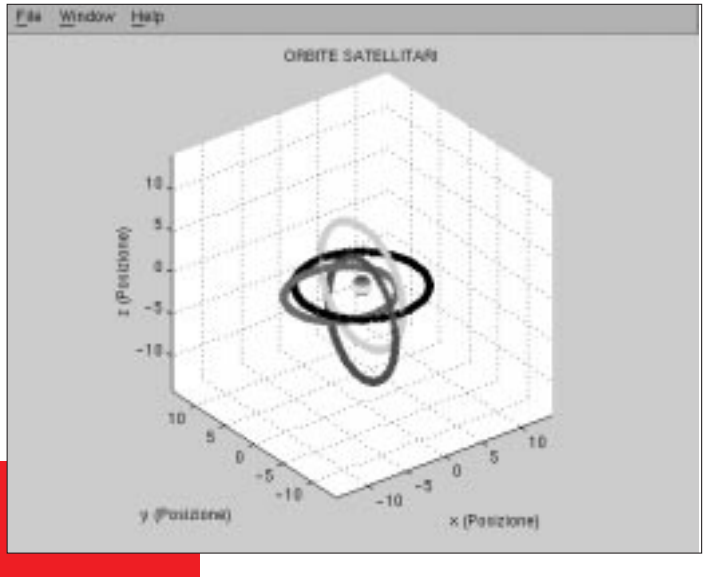

Figure 1: *Satellite orbits (A. Canziani, G. Isella and M. Sampellegrini, Istituto Tecnico Industriale "L. Cobianchi" Verbania, Italy).*

1. Camp Organization

The camp is jointly organized by CSCS/SCSC, the Swiss Group "Ingenieure für die Schweiz von morgen" (INGCH) and the Department of Education and Culture of the Canton of Ticino, with the collaboration of the local University of Applied Sciences (SUPSI) and the Lugano based "Istituto Dalle Molle di Studi sull'Intelligenza Artificiale" (IDSIA). Financial support is provided by CSCS/SCSC, ETHZ, those Swiss cantons with students participating in the camp and a consortium of firms interested in supporting educational programs.

The main objective of the camp is to give gifted high school students the theoretical and practical background of computer simulation using state-of-the-art technologies and equipment. The ever growing importance of computer simulation in the different scientific disciplines is demonstrated and emphasized, opening new perspectives to the camp participants for their further education at academic or professional level.

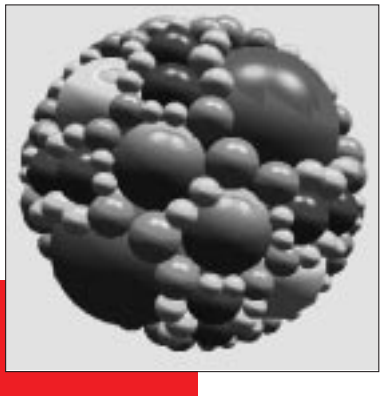

Figure 3: *Raytracing technique (W. Strauss, Gymnasium Köniz, Bern).*

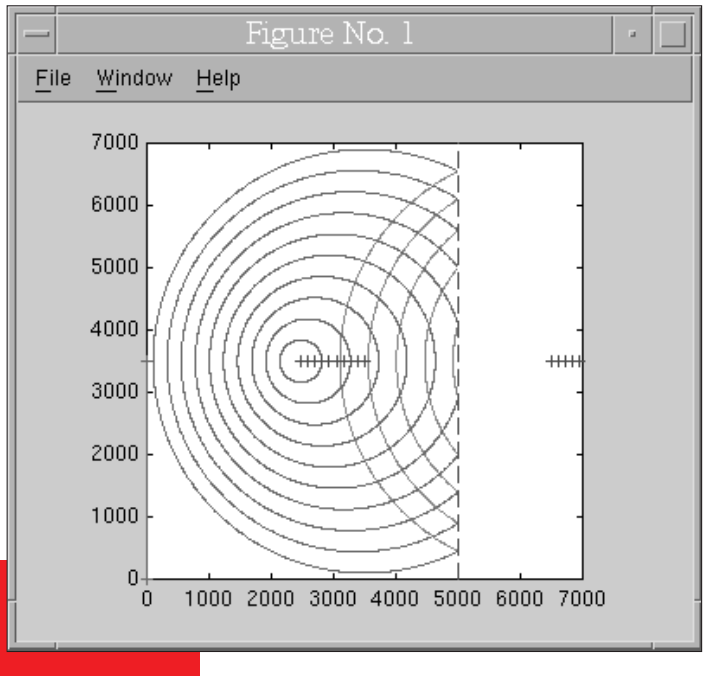

Figure 2: *Doppler effect (P. Jermini, Liceo Bellinzona, Ticino).*

The camp was held this year in two sessions of two weeks each, with the same program repeated in each session:

- 1st Session: July 12 - July 25
- 2nd Session: July 26 - August 8

Fifteen students were selected in the first session and twenty-one in the second session (of which four students finally could not participate), with a final total of thirty-two participants.

Figure 4: *Discussions during the press conference aperitif. From left: A journalist and Mrs. M. de Senarclens (INGCH), assistants T. Burg, A. Gerszt and B. Lutz, Prof. H.-P. Frei (UBS) and B. Zumthor.*

Figure 5: *Rafting on the Ticino river.*

The geographic origin of the participants was the following: twelve from the German-speaking part of Switzerland, seven from the French-speaking part of Switzerland, one from the Canton of Ticino and twelve from the Italian "Regio insubrica."

2. Camp Activities

The first days of the camp were dedicated as always to introductory lectures given by experts from either CSCS/ SCSC or one of the specialized partner institutions. The topics of these lectures were: scientific simulation, Unix, networks, Internet and Web, mathematical software packages (Maple and Matlab), artificial intelligence, and scientific visualization.

The working language of the camp is English, acting as a common language of interaction between the participants and with the instructors. Although not all participants had a fluent usage of the language, mutual understanding was sufficient and many students saw this as a welcome training. The various other national languages were also used where necessary or convenient.

The remainder of the camp was dedicated to the realization of the simulation projects the students had proposed as part of their camp application; the work was followed and supported by assigned advisors and assistants. The advisors are experts in various project application fields, coming from CSCS/ SCSC or external partner institutions, while the assistants are university students who had been former C^3 participants and have the important role of help and interface persons experienced in the camp environment.

The project fields were varied and included physics (trajectories of flying objects, light propagation, Doppler effect), astronomy (solar system, asteroid collision, satellite orbits),

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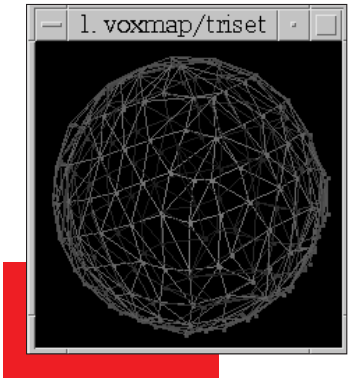

Figure 6: *Representation of isosurfaces (C. Bény, Gymnase de Nyon, Vaud).*

materials science (structure of minerals), fluid-dynamics (Zeppelin airship simulation, surface construction), system theory and artificial intelligence (intelligent traffic control systems, Bongard problems, intelligent computer player, cryptographic systems based on fractals), finance (portfolio management) and visualization (raytracing, landscape representation). Remarkable this year was the proposal and realization of the first C³ project in the field of finance. The complete documentation on participants and projects can be found on the Web pages ("www.cscs.ch/C3").

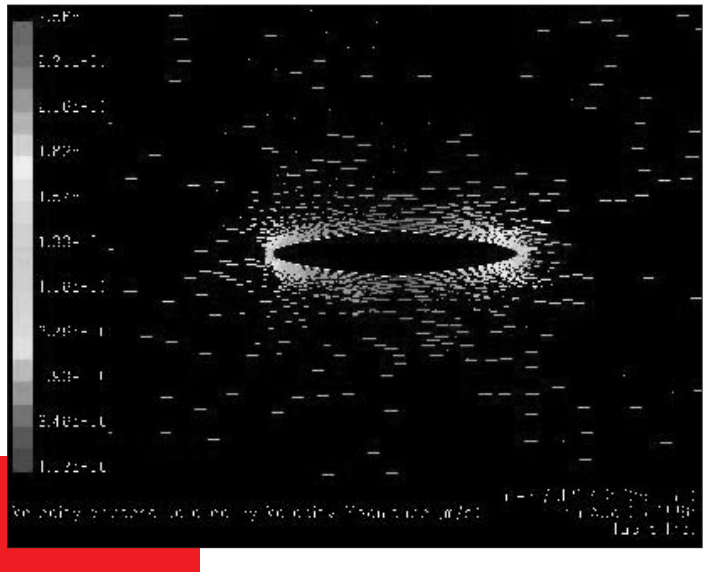

Figure 7: *Zeppelin airship simulation (D. Perler, Collège de Gambach, Fribourg).*

Besides the lectures and the project activity there were planned recreational activities on Saturdays, including an amusing and exciting rafting down the river Ticino from Claro to Bellinzona.

In conclusion we can say that the C³ was a success once again, with a good media coverage (all Ticino newspapers, some Swiss magazine, Ticino radio and TV).

A hearty thanks for the support and the cooperation goes to all persons and institutions involved in the organization and realization of the camp, namely the advisors and assistants, the sponsors, the CSCS/SCSC management and staff.

Contact
Bernardo Zumthor (bzumthor@cscs.ch) ■

CSCS/SCSC Technical Reports 1998

TR-98-01 *Abelian Projection without Ambiguities.*
A. J. van der Sijs (February 1998)

TR-98-02 *Topological Properties of the QCD Vacuum at $T = 0$ and $T \sim T_c$.*
Ph. de Forcrand, M. Garcìa Pérez, J. E. Hetrick, and I.-O. Stamatescu (February 1998)

TR-98-03 *High-T_c Superconductivity through a Charge Pairing Mechanism in a Strongly Coupled Disordered Phase.*
J. L. Alonso, Ph. Boucaud, V. Martín-Mayor and A. J. van der Sijs (April 1998)

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Report on Supercomputing '98, Mannheim

Djordje Maric (CSCS/SCSC)

The European "Supercomputing 98" conference took place in Mannheim (Germany) on June 18-20. The simultaneous publication of the biannual TOP500 list attracted much attention. The second release in autumn coincides with Supercomputing USA.

Among the invited speakers were Dr. Geiger (Director of HLRS in Stuttgart), Dr. Hegering (Director of Leibniz Center in Muenchen), Dr. Hossfeld (Director of Center in Jülich), Dr.Neves (Director of IT at Boeing) and Dr. Smarr (Director of NCSA). Dr. Maric delivered a talk entitled "Obtaining High Sustained Performance with Real-life Applications at CSCS-ETHZ". The invitation to present at Supercomputing '98 is an international recognition for the results of the NEC-CSCS Joint Collaboration in Applications Porting and Optimization on the NEC SX-4 in Manno. It has also provided the opportunity to compare CSCS/SCSC PVP HPC services on an international scale—with excellent results. CSCS/SCSC PVP HPC services are among the best offered in HPC production centers.

For a copy the conference proceedings and/or additional information, please contact Dr. D. Maric at dmaric@cscs.ch.

Contact
Djordje Maric (dmaric@cscs.ch)

Report on the WWW7 Conference

The Seventh International World Wide Web Conference took place in Brisbane (Australia) from April 14-18, 1998. The conference days were composed of a tutorial/workshop day, a developer's day and three days of "traditional" conference days. CSCS/SCSC's Ivan Pontiggia was amongst the approximately 1,400 participants.

As in years past, Tim Berners-Lee, father of the world wide web and director of the World Wide Web Consortium (W3C), addressed the conference delegates with a keynote address. The theme of his address was this year's hot new development: the Resource Description Framework (RDF). RDF provides a generic framework for metadata on the Web (providing "data about data") and is considered to be the (up to now) missing architectural web component; RDF complements the flexibility found in addressing (URLs), transport (HTTP) and data format (XML). W3C is focussing its current initiatives around a building a semantic web that can be trusted and RDF is a major part of this initiative. Other associated initiatives include digital signatures, rating schemes and privacy applications.

The need for reliable and detailed metadata for resource discovery is becoming more and more important as can be witnessed by the submitted papers: approximately 20% were concerned with information retrieval and 17% were concerned with search and indexing techniques. It should also be noted that there was a large librarian presence amongst conference participants. RDF could be an important step in making embedded metadata more reliable—critical for automated search engines and application in subject gateways.

The next conference will be held in Toronto, followed by Amsterdam.

Fourth World Conference and Exhibition in Applied Fluid Dynamics of the World User Association in Applied Computational Fluid Dynamics (WUA-CFD)

Stefan Haberhauer and René Hausammann (NEC-European Supercomputer Systems)

The Fourth World Conference and Exhibition in Applied Fluid Dynamics was held June 7–11, 1998 in Freiburg (Germany). The conference attracted more than 180 engineers and researchers from all over the world. The attendees, about three-quarters representing companies, were diverse in backgrounds and perspectives of CFD: some were developing their own simulation codes while others—especially those from industry—were using commercial applications.

From the many topic areas quite a few presentations were related to the verification of computer-based simulations by experiments and vice versa. While some researchers ask for even higher accuracy, most engineers from industry concentrate on efficient simulations to provide sufficiently accurate solutions within the rigid boundaries of time and budget. During discussions, the need for establishing well-defined standardized test cases with verified experimental data was considered crucial for quality assurance and for comparison of the power and reliability of the various simulation packages.

Another important topic focused on mesh generation and automatic optimization which today is still a process demanding significant manual interaction and much experience.

CSCS/SCSC was present at the exhibition as a partner in the NEC booth. The Task Force projects related to CFD were presented in detail on posters. These projects were the porting of a multiblock Navier-Stokes solver (NSMB) to the message-passing standard MPI (Dr. J. Vos, EPF Lausanne) and the two projects related to turbulence modeling based on Direct Numerical Simulation in collaboration with the groups of Prof. Deville (EPF Lausanne) and Prof. Kleiser (ETH Zurich) which exploit shared memory parallelization based on microtasking. Besides the posters, a video of scientific animations produced by the CSCS/SCSC visualization group was shown and attracted attendees to stop, watch and discuss. NEC presented the newly introduced SX-5 system, which boosts the overall system performance by a factor of four compared to an equally sized SX-4, the system currently installed at CSCS/ SCSC (Manno).

The increasing demand for such powerful and affordable systems was shown in a very impressive way by three-dimensional interactive visualization and is driven even further by the request for multi-physics-approaches (e.g., fluid-structure interaction) and automatic optimization.

NEC whishes to thank the individuals involved in the preparations for this exhibition, with special thanks to Angelo Mangili, Silvia Walther, Jean-Pierre Therre and to the research groups of Prof. Kleiser, Prof. Deville and Dr. Vos for their support.

A comprehensive overview of all the projects in CSCS/SCSC-NEC Joint Collaboration on Application Porting and Development can be found on-line (http://www.cscs.ch/Official/Services/TaskForce/) or can be requested in printed form from the NEC Branch Office of Manno.

Contacts
Stefan Haberhauer (shaberhauer@nec.ch)
René Hausammann (rhausammann@nec.ch) ■

A User Project: First-Principles Calculation of Electric-Field Gradients at the Cu Sites in the High Temperature Superconductor $YBa_2Cu_3O_7$

P. Hüsser, S. Schafroth, E. Stoll, H.U. Suter, and P.F. Meier (Department of Physics, University of Zurich)

As a step towards understanding the basic mechanisms of high-temperature superconductivity, the electric-field gradients at the Cu sites in $YBa_2Cu_3O_7$ have been investigated using first-principles cluster procedures. For the planar Cu, a large cluster comprising 74 atoms was studied with both Hartree-Fock and density functional methods. The latter calculations provide field gradients and asymmetry parameters in good agreement with the experimental values for hydrostatic pressures up to 0.6 GPa.

1. Introduction

Superconductivity is a solid state phenomenon based on quantum mechanics. Two electrons with opposite internal rotation (called spin), moving through the system with an energy close to the Fermi energy, are bound due to the action of lattice vibrations and together form a Cooper pair [1]. These pairs travel unimpeded by scattering through the system. Therefore, superconductors can transport the electric current without losses. Substances that become superconducting do so only below a certain temperature, called the critical temperature T_c, which varies from substance to substance. For "classical superconductors" such as simple metallic elements this tends to be approximately of the order ten Kelvin; for metallic lead T_c = 7.22 K. In 1986 Müller and Bednorz [2] discovered that certain copper oxide compounds remain superconducting at much higher temperatures (T_c = 30 ... 130 K); these substances are called high-temperature superconductors. Although the basic mechanism of metallic superconductors has been known since 1957 [1], efforts so far have been unsuccessful in explaining a conclusive theory for the occurrence of superconductivity in copper oxides. One step towards the understanding of this phenomenon is to calculate by quantum mechanics the states of the conduction electrons of such complicated compounds. To test the computation validity, these results must be compared with corresponding experimentally accessible solid state properties.

Such data can be obtained with nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) spectroscopy. These methods provide a considerable amount of information on both static and dynamic properties of high-temperature superconductors. The resonance frequencies of the nuclear magnetic moments in an applied external magnetic field are directly proportional to the change of the electric field at the location of the investigated atom core. This electric field gradient (EFG) has been determined for a variety of nuclei with high accuracy [3].

2. Computer Simulations of Electronic Properties

Ab initio quantum chemical computer simulations determine the charge distribution of all electrons in the environment of the considered atoms. The contributions of the electronic charge to the EFG decay with $1/R^3$ where R is the distance from the observed atomic center. This power law emphasizes the contributions from all electrons close to the core. The EFG depends closely to the precise distribution of the copper *d*-electrons that are responsible for the electric conductivity and superconductivity and are concentrated very close to the Cu atom center.

One reason for the extreme difficulty of electron property calculations is the rather complicated crystallographic structure of high-temperature superconductors, as plotted in Figure 1a. The unit cell contains several different types of metal atoms (Y, Ba, and Cu) as well as oxygen atoms. There are two types of Cu atoms: Cu(1) with two O as neighbors and Cu(2) with four

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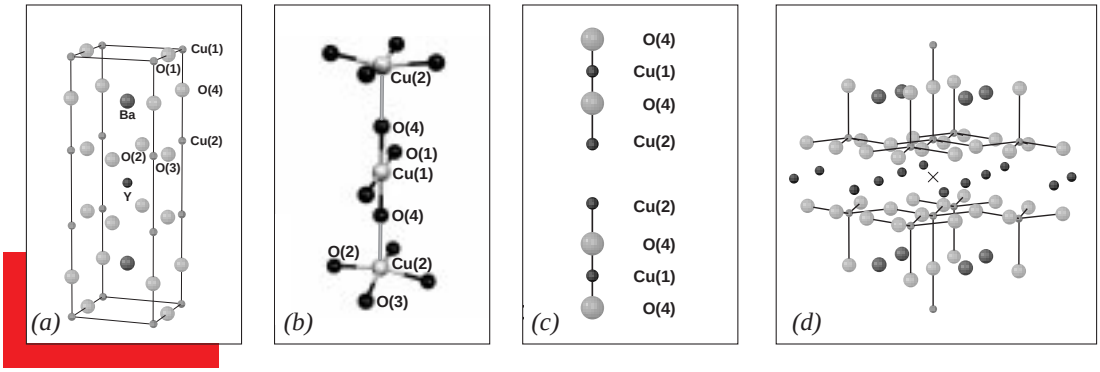

Figure 1: *(a) Unit cell of the $YBa_2Cu_3O_7$ high-T_c superconductor. (b) Cu_3O_{12}-cluster for the calculation of the EFG on the Cu(1) atom. (c) Chain of the Cu and oxygen atoms in the $YBa_2Cu_3O_7$ system perpendicular to the mirror plane denoted by the piercing point M [7]. (d) The $Cu_{12}O_{42}Y_{12}Ba_8$ cluster[7]. 12 Y atoms are in the middle plane. Cu (small) and O (large) atoms are connected with lines. The remaining dark balls denote the Ba atoms.*

(Continued from page 15)

neighboring O in a plane and one O, O(4) in the apex. This complex material has properties of an ionic crystal and simultaneously those of a metal.

The origin of the electrical conductivity (of Cu) is much more difficult to understand than in simple metals such as sodium [4, 6], magnesium [5, 6] or aluminum [4, 6]. For all atoms, the electrons are attracted by the positive core and localized in shells. This attraction is rather large for the most inner shells with a large and negative binding energy. These electrons shield the remaining electrons in the outer shells against the electrostatic core forces. Therefore, the binding energy of the electrons becomes weaker and weaker the further away from the core their shells lie. In simple metals the electrons with energies close to the Fermi energy are bound so loosely that they can move almost freely through the whole metallic bulk and the nuclear attraction can be treated as a small perturbation (Figure 2 a).

But things become much more difficult in the copper atoms of high-temperature superconductors when the *d*-electrons contribute to the electrical conductivity and superconductivity. The spatial distribution of the *d*-electrons in the atoms resembles those of seeds in an apple and they are located rather close to the core (Figure 2b). But their energy close to the Fermi energy is higher than that of the farther extending shells. Instead of the more negative electrons shielding those with higher energy, the electrons with the higher energy shield those with the lower energy. This complex situation has consequences on the convergence for computer simulations. The electron self-shielding can only be calculated iteratively. This shielding depends on the electron density distribution and alters the potential energy acting on the electrons. To compute the charge distribution the wavefunction eigenvalues must be determined by solving the electron eigenvalue problem. The corresponding matrix elements depend on the electron potential energy. Starting with an arbitrary electron distribution, the first correction to the electron density is calculated. With this correction the shielding and the potential energy are then recalculated and these updating cycles are repeated as long as the changes of the total energy are larger than a given threshold. For simple metals and simple semiconductors (such as silicon with *s*- and *p*-electrons at the Fermi-energy) this self-consistent computation converges very quickly. A much more complex situation occurs in the high-temperature superconductors. Here, at the Fermi-energy we have a wavefunction mixture of very localized Cu *d*-electrons and expanded oxygen *p*-electrons. A reasonable amount of electric charge can be moved with each computation cycle. The convergence behavior therefore is poor, and it is difficult to find a monotonically descending path in the energy landscape that tends towards the absolute minimum and that avoids too close approaches to relative maxima and saddlepoints. This very involved behavior of the conduction electrons also prevented the correct calculation of the electronic Cu-Cu interaction in the interpretation of one of the first inelastic neutron scattering results on pure copper metal [8].

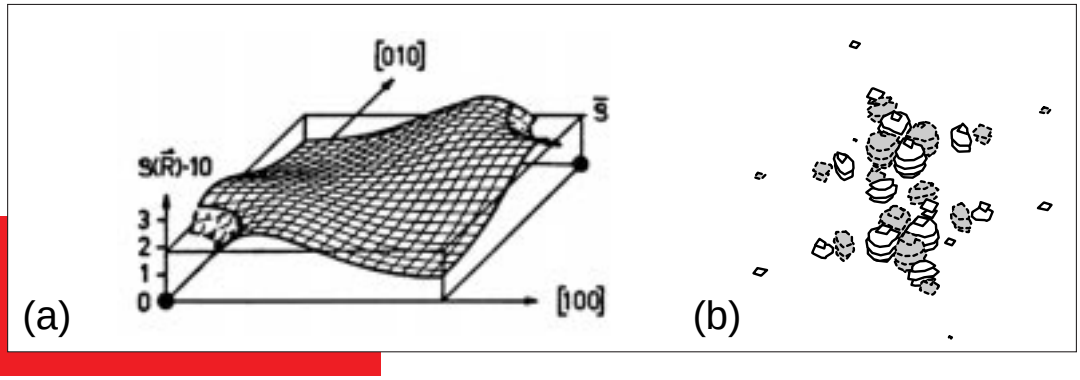

Figure 2: *(a) Density of the 2s and 2p conduction electrons in aluminum [6]. (b) Highest occupied molecular orbital in $YBa_2Cu_3O_7$ [7]. The shadowed regions indicate negative sign. The square of this wavefunction corresponds to the density of the oxygen 2p and copper 3d conduction electrons.*

Electrons interact directly via their electrostatic repulsion. Furthermore, the Pauli principle forces electrons with the same internal rotation or spin direction to repel each other, and this electron exchange is the basis of the Hartree-Fock (HF) method. The electrostatic repulsion also excludes a close approach of electrons with different internal rotation or anti-parallel spins. This electron correlation together with the exchange are considered in the density functional (DF) methods.

Earlier calculations of the EFGs at the Cu(2) site [9, 10] failed to predict the experimental value [11]. We recalculated the EFGs by using appropriate large clusters and more suitable basis sets. The simulations were performed with the Gaussian 94 [12] program package on the CONVEX Exemplar and on the NEC SX-4 computers at CSCS/SCSC in Manno. The DF methods were applied using both the local density approximation (LDA) [13] and the generalized gradient approximation (GGA) [14] and compared with HF calculations.

To determine the electric field gradients at a specific lattice site it is necessary to choose a cluster that is centered appropriately. For the Cu(1) site in $YBa_2Cu_3O_7$, calculations with a rather small cluster (Cu_3O_{12}), shown in Figure 1b, yield EFGs in good agreement with the experiments. For Cu(2), however, a considerably larger cluster ($Cu_{12}O_{42}Y_{12}Ba_8$) is needed. It contains 74 atoms and is centered around the midpoint (Figure 1c) between two adjacent Cu(2) sites along the c direction (Figure 1d). This cluster has zero charge and is, in addition, embedded in 2448 point charges simulating the ionic environment.

3. Results

method	Cu(1) V_{bb}	η	Cu(2) V_{cc}	η
UHF[a]	11.2	0.3	-22.2	0.04
LAPW[b]	7.4	0.8	-5.6	0.07
HF[c]	28.53	0.04	-20.73	0.09
DF/LDA[c]	7.49	1.00	-15.76	0.00
DF/GGA[c]	7.12	0.94	-16.17	0.01
experiment[d]	7.51±0.03	0.99	-12.35±0.02	0.01

Table 1. *Theoretical and experimental EFGs (in 10^{21} Vm^{-2}) and asymmetry parameters at Cu(1) and Cu(2) in $YBa_2Cu_3O_7$. a) [9], b) [10], c) [7], and d) [11]*

The calculated EFGs at the Cu sites obtained with HF and the DF methods are given in Table 1, together with previous theoretical values and experimental data [11]. For Cu(1), our EFG values calculated with DF are in agreement with previous theoretical studies. For Cu(2) [7], the EFGs calculated with DF are closer to the experimental value than those obtained with earlier theoretical approaches [9, 10]. (The suppression of the electron correlation in HF leads to a less reliable result.)

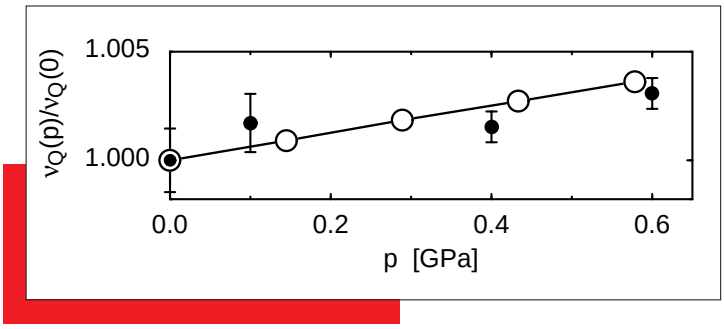

Figure 3: *Normalized pressure dependent NQR frequencies $\nu_Q(p)/\nu_Q(0)$.* ● *experiments of Ref. [16].* ○ *our DF/GGA calculations [17].*

Furthermore, the pressure dependence of the EFG at the Cu(2) site was determined by varying the lattice parameters [15]. This simulation of the influence of hydrostatic pressure is in good agreement with NQR experiments [16] (Figure 2).

4. Summary and Conclusions

Using first-principles cluster procedures the electric-field gradients at the Cu sites in $YBa_2Cu_3O_7$ have been investigated. For the symmetrical Cu(1) between the chain oxygens our results correspond to those of earlier calculations [9, 10] and describe the experimental value [11] well. For the planar Cu(2), a large cluster comprising 74 atoms was studied with both Hartree-Fock and density functional methods. The latter calculations provide field gradients and asymmetry parameters in good agreement with the experimental values [11]. Such a good agreement was also found for the EFGs at the Cu(2) site for hydrostatic pressures up to 0.6 GPa.

Acknowledgments

We would like to thank D. Brinkmann, M. Hodous, M. Mali, C. Moor-Häberling, and J. Roos for valuable discussions. This work is partially supported by the Swiss National Science Foundation. We thank the CSCS/SCSC in Manno for hospitality during the Project Related Student Stages in Summer 1995 and for its support.

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Contacts

Peter Hüsser (huesser@physik.unizh.ch)

Stefan Schafroth (schafrot@physik.unizh.ch)

Erich Stoll (stoll@physik.unizh.ch)

Hans Ulrich Suter (suter@physik.unizh.ch)

Peter F. Meier (pfmeier@physik.unizh.ch) ■

CSCS/SCSC Contributes to the Swiss-Tx Commodity Parallel Supercomputer Program

Karsten M. Decker (CSCS/SCSC) and Ralf Gruber (SIC-EPFL)

Introduction

Responding to the rapidly changing situation in the supercomputer market, and following a thorough analysis of high-performance computing related programs in the U.S.A., EPF Lausanne has initiated the Swiss-Tx commodity parallel supercomputer program in September 1997 [1]. The goal of Swiss-Tx project is to realize and practically demonstrate a parallel, commodity component-based computer system with a peak performance of more than 1 TFlop/s in the first quarter of the year 2000. This goal will be achieved by successively developing four increasingly powerful, scalable parallel processor prototype systems built from standard Digital Alpha processor boxes (one, two or four processors with shared memory, disks, PCI interface, operating system, standard compilers and libraries), interconnected with a novel interconnection technology from Supercomputer Systems AG (SCS), Zurich. The first prototype, called *Swiss-T0*, with eight Digital Alpha 21164 processors has already been installed at and accepted by EPF Lausanne. The second prototype, the *Swiss-T0(Dual)* will be installed in October 1998.

The Swiss-Tx project is managed by a six member board: three from EPF Lausanne, one from Compaq, one from ETH Zurich and one from SCS. The hardware for the Swiss-Tx project and part of the user support are sponsored by Compaq, while the Swiss Commission for Technology and Innovation (CTI) provides financial support for software development, application porting, benchmarking and evaluation, and part of the user support.

The Project Partners

The Swiss-Tx project is a large-scale collaborative effort, exploiting the extended expertise of groups in Switzerland and the U.S.A. The following institutions and organizations are committed to the effort.

IFE-ETHZ (Institute for Electronics). Development of the 12 x 12 crossbar interconnection technology and the communication libraries FCI, MPI-lite, and MPI. The responsible person is Prof. Anton Gunzinger.

CSCS/SCSC (Swiss Center for Scientific Computing). Provision of a portable, extensible, and customizable environment, accessible from any desk-top environment over the network, to support programming of new applications, (performance) engineering of existing applications, and management of running applications on parallel and distributed platforms. CSCS/SCSC has been invited to join the project because of its demonstrated experience in tools development for parallel and distributed systems with academic and industrial partners over the last five years [2]. The responsible person is PD Dr. Karsten M. Decker.

SIC-EPFL (Service Informatique Central). Provision of basic resource management functionality such as user validation, resource allocation, system partitioning, job scheduling, checkpoint/restart, system performance monitoring and tuning, archiving, and accounting. SIC has more than ten years experience in managing vector and parallel machines such as the Cray-1, Cray-2, Cray-YMP, Cray-T3D, and SGI Origin-2000. The responsible person is Michel Jaunin.

CAPA-EPFL (Centre pour les Applications Parallèles et Avancées). Test and evaluation of the Swiss-Tx series of parallel computer systems, comprising function tests, performance evaluation, and porting and optimizing of full-scale applications from the Laboratoire en Mécanique des Fluides, the Centre de Recherche en Physique des Plasmas, the Institut Romand de Recherche Numérique en Physique des Matériaux, and the Institut de Mesures et Analyse des Contraintes. The responsible person is Dr. Ralf Gruber.

LSP-EPFL (Laboratoire des Systèmes Périphériques). Development of the high-level parallel file system library based on the existing Parallel Storage and Processing System (PS^2). Porting and adaptation of the Computer-Aided Parallelization (CAP) software to the Swiss-Tx machines to ease use of the parallel and distributed file system. The responsible persons are Prof. Roger Hersch and Dr. Benoit Gennart.

LITH/GRIP-EPFL (Laboratoire d'Informatique Théorique/ Groupe de Recherche en Informatique Parallèle). Porting and adaptation of an I/O-intensive application to the Swiss-Tx series of parallel computer systems. This application will be used to test and evaluate the distributed I/O system. The responsible persons is Dr. Pierre Kuonen.

DMA-EPFL (Département de Mathématique/Chaire d'analyse appliquée). Development of parallel data representation, data reduction and visualization techniques for the interactive control of parameter continuation computations. The responsible person is Prof. John Maddocks.

SCS AG (Supercomputing Systems, Zurich). Assembly and testing of the four scalable parallel processor prototype systems, installation at EPF Lausanne, and system support. In addition, SCS will realize the interconnection networks for the four Swiss-Tx prototype systems and will collaborate with IFE-ETHZ to implement the FCI, MPI-lite, and MPI communication libraries. The responsible person is Martin Frey.

Compaq. Provision of hardware components (processors, memory, disks) and basic software (Digital UNIX and Windows/NT operating systems, compilers and mathematical libraries) at largely discounted prices. In addition, Compaq assigns one full-time system analyst to support Digital UNIX and Windows/NT and establish direct contacts with the specialists at Compaq as required. The responsible persons are Dr. William Blake, Dr. Ivan Sipos, Dr. Martin Walker and Galip Ozem.

Oracle. Port of the Oracle parallel data base management system to the Swiss-Tx series of parallel computer systems. The responsible person is Dr. Dols.

SNL (Sandia National Laboratory). Engineers and scientists from SNL will test and evaluate the Swiss-Tx series of parallel computer systems, while engineers from EPF Lausanne will evaluate the parallel systems being built at SNL. The systems developed at SNL are also based on Digital Alpha processors but use the Myrinet interconnection technology from Myricom. The responsible person is Dr. William Camp.

ORNL (Oak Ridge National Laboratory). Engineers from ORNL will contribute to the testing and evaluation of the Swiss-Tx series of parallel computer systems, while engineers from EPF Lausanne will evaluate the SRC machine to be installed beginning 1999 at ORNL. The responsible person is Dr. Kenneth Kliewer.

McKinsey Partner. McKinsey Partner will help to create a spin-off company to produce, market and sell the Swiss-Tx series of parallel computer systems. The responsible person is Sauro Nicli.

Conclusion

The Swiss-Tx project gives Switzerland the unique opportunity to build its own affordable commodity supercomputers by collecting and exploiting the huge existing knowledge in HPC available in the country. The strong involvement of Compaq in this project offers the possibility to install at a low price a Teraflop machine in Switzerland by the year 2000. A spin-off company will be created to start commercializing the crossbar connected Swiss-T1 and Swiss-T2 machines in 1999.

References

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[2] K. M. Decker. I²A-CSCS/SCSC Software Technology Projects. http://www.cscs.ch/Official/SoftwareTech/, October 1998. CSCS/SCSC, CH-6928 Manno, Switzerland.

Contacts
Karsten M. Decker (decker@cscs.ch)
Ralf Gruber (Ralf.Gruber@epfl.ch) ■

Jean-Pierre Therre Resigns—Hans-Peter Wessels Director Ad Interim

Jean-Pierre Therre, director of CSCS/SCSC since 1996, resigned as of August 27, 1998.

The Center is directed *ad interim* by Dr. Hans-Peter Wessels.

Hans-Peter Wessels was born in 1962 and graduated with a Ph.D. in biochemistry from the University of Basel. Since 1997 he is assistant to the Vice President for Research of the Federal Institute of Technology of Zürich (ETHZ). ■

JULIUS PROJECT - ESPRIT 25050: JOINT INDUSTRIAL INTERFACE FOR END-USER SIMULATIONS

John Murphy (British Aerospace Ltd., Sowerby Research Centre), David Rowse (British Aerospace Ltd., Sowerby Research Centre), Luciano Fornasier (Deutsche Aerospace AG), Philippe Thomas (Dassault Aviation), Argiris Kamoulakos (Engineering Systems International) and Edgar A. Gerteisen (CSCS/SCSC)

Julius is embedded within the Fourth Framework Programme, RTD in Information Technologie Domain 6, HPCN Simulation and Design, Primarily Task 6-3. Julius is a joint activity of industrial end-users and of software developers (called technology providers) for the development of a standard framework for customization of problem-solving environments. Although the end-user partners themselves are carrying out some of the developments, one of their central roles is to provide input to the specification of end-user requirements and tool evaluation. These industrial end-users, represented by British Aerospace (BAe), Daimler Benz Aerospace (DASA), Dassault Aviation and Engineering Systems International (ESI), steer the project and bring in requirements from the automotive and manufacturing sectors. The software developers are Genias, Fraunhofer Institut für Produktionsanlagen und Konstruktionstechnik (IPK), Numerical Algorithms Group (NAG), University of Oxford (OUCL), University of Swansea (UWS), CSCS/SCSC and Stehlin-Merazzi Research (SMR).

Introduction

The complexity of today's engineering simulations demands the use of many HPCN and engineering simulation tools by end-users. All of these tools need to be accessible to the engineer and, ideally, in a seamless environment. Simultaneously, issues such as time-to-market demand significant reductions in design time as product complexity increases. Consequently the end-user engineer has an extremely complex simulation system to control, both the hardware and the software, and the human productivity needs to increase to achieve order of magnitude reductions in design time for many applications.

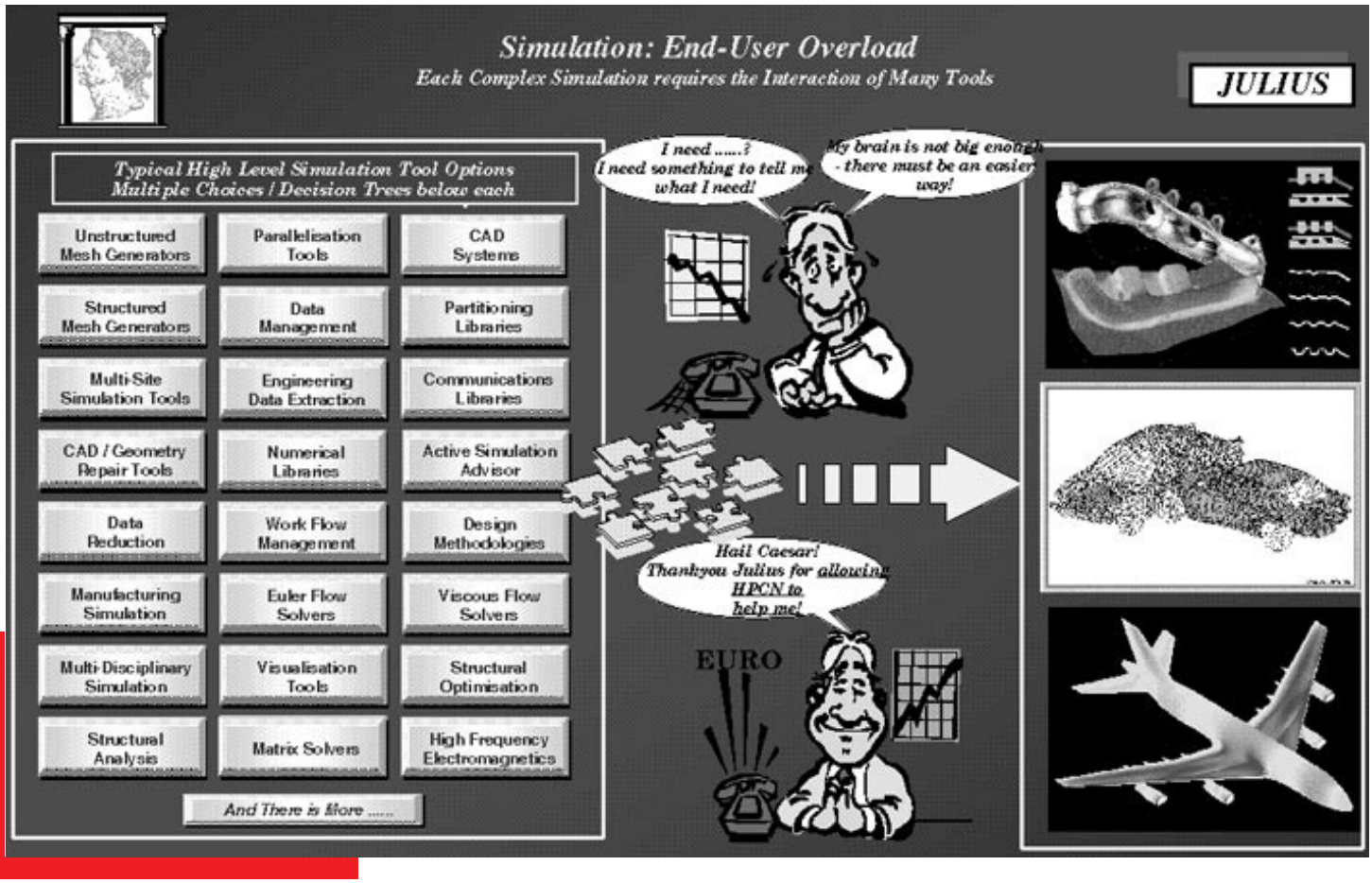

Figure 1: *End-user engineer overload*

The increased performance and lower prices of HPCN platforms enables the required growth in simulation across many industrial sectors to help address the above issues. However, the fuller benefits of these HPCN systems can only be realised if greater efficiency is introduced into the end-user interfaces for pre- and post-processing, particularly as the volume of data increases with the growth in simulation complexity. The multitude of tools needed for a single complex simulation brings bottlenecks and limitations associated with tool interaction, and data transfer. These bottlenecks must be prioritised and addressed to provide HPCN assisted pre- and post-processing, essentially redistributing the workload between the end-user and the HPCN platform, allowing the end-user to focus more creatively on design goals.

The requirements of many engineering-based companies, reflected in the project by major European aerospace partners and by ESI, relates to addressing increasingly complex products and reducing the cost and the length of the design cycle. These two factors require substantial increases in design effort from year to year. As an example, a wing design for a European civil aircraft required the computer simulation of 800 design options. The computer analyses were carried out over two years. To reduce this to three months for future aircraft (with added complexity) will require an order of magnitude increase in design effort. Consequently, the objective of this project is:

- to develop an integrated functional HPCN environment for simulation in multiple disciplines,
- to provide and demonstrate HPCN tools and engineering simulation tools that will efficiently work together in this environment,
- to put developments in place to remove the main limitations and bottlenecks in engineering simulation, prioritised by the industrial end-user, and
- to demonstrate the entire system working with embedded applications software for real industrial problems including multi-site cooperative working.

The environment is called 6S Environment (6S being an abbreviation for Sixth Sense). It will have an open modular structure to enable the use of tools and applications software from alternative suppliers. The backbone of the project is an industrial test case suite, which is agreed by the industrial end-users and is derived primarily from the final industrial demonstrators. This will steer the technical developments and enable the end-user industries to evaluate the developments and provide feedback throughout the project. The starting point for the 6S environment is the Parallel Simulation User Environment (PSUE) developed and successfully demonstrated in the CAESAR ESPRIT project but with limited application. The developments here provide a more seamless simulation and design environment with advanced engineering simulation tools including CAD repair and control facility, an integrated grid generation capability and active engineering advisor modules to monitor and help the end-user.

The project provides a number of tools suitable for commercial exploitation. 6S will come in three forms—the complete version (6S-C), the developer's version (6S-D) and the end user version (6S-E); each version will have a 'preferences' feature. The grid generation capability and the CAD repair capability are also suitable for commercialisation as well as an enhanced dynamic version of CODINE. Throughout the project, four versions of the 6S Environment + Tools will be released. These deliverables are expected to provide significant benefits to the industrial end users and many are innovative.

6S and JULIUS Developments

The developments aim at achieving a balanced simulation environment so that end-users can focus on engineering design goals rather than the complexity of the simulation software and hardware. Engineering business requirements demand an order of magnitude improvement in computational design effort per unit time for a number of applications. To achieve this it is necessary to identify the bottlenecks, many of which lie in the area of pre- and post-processing, and exploit HPCN to increase human productivity. This work was started in the CEASAR ESPRIT demonstrator project with the development of a prototype integrated computing environment for multiple disciplines, called PSUE. The project successfully demonstrated that significant reductions in pre-processing could be achieved for the applications considered. Within JULIUS, the CEASAR PSUE is extended from its prototype, demonstrator level to a more robust and operational state, with associated developments that broaden the applicability to a range of simulations defined by industry and represented in the demonstrator suite.

The project is driven by full industrial demonstrators defined by the end-user industry partners. These are examples of real industrial problems that must be solved within their businesses. Important to note is that all these demonstrators are inherently multi-disciplinary in nature, demanding the coupling of electromagnetics (EM) with structural mechanics

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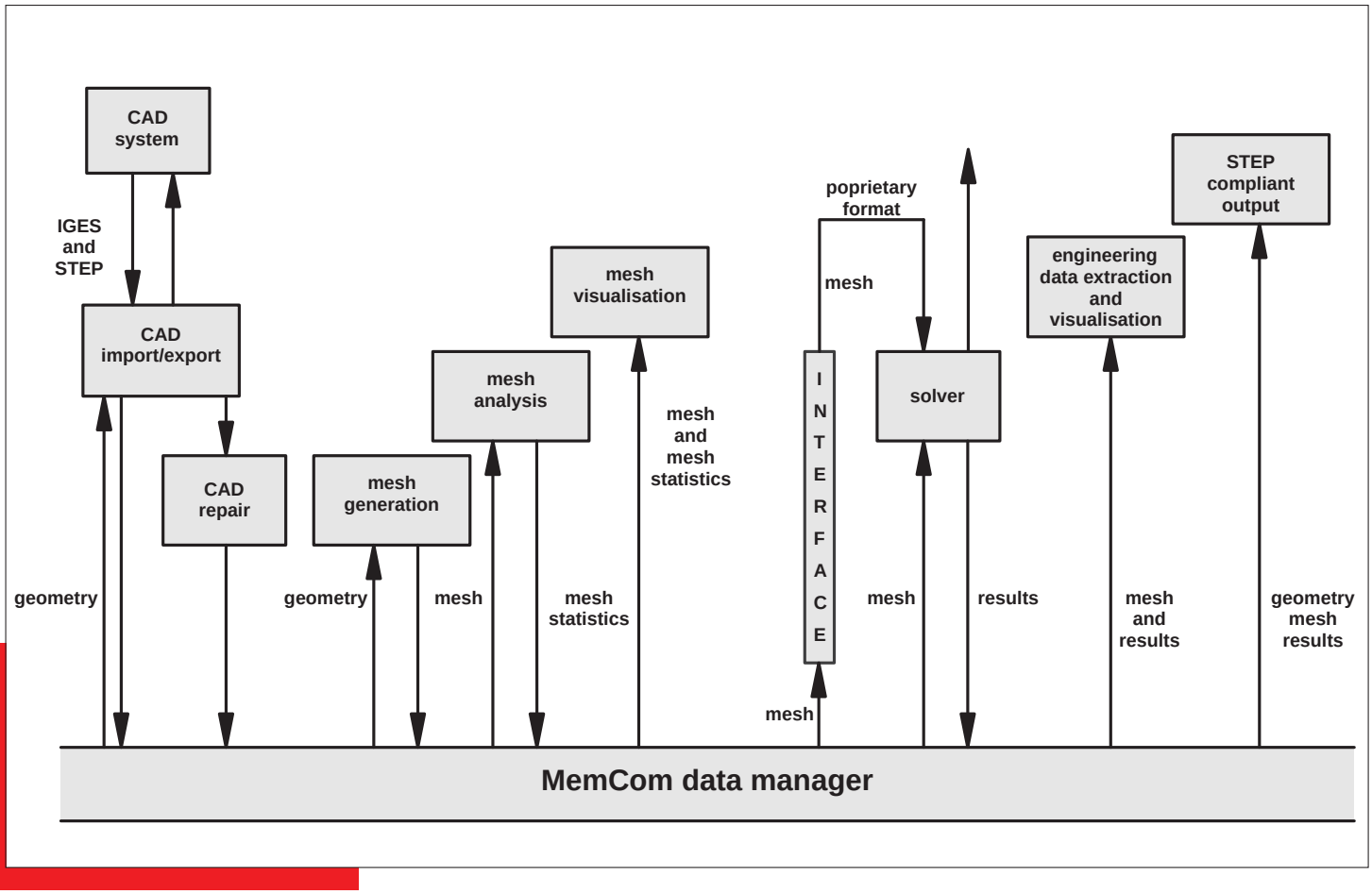

Figure 2: *Data flow schematic for 6S environment*

(CSD), computational fluid mechanics (CFD) with CSD and optimization routines, together with dynamic geometry modification, and subsequent mesh generation and adaptation. These demonstrators are selected to reflect the main challenges in moving engineering simulation forward.

The complexity of these simulation tasks requires the integration of a number of tools and applications software that come from different suppliers. The data flow through 6S via common standard data objects and access functions is regarded an essential feature for the realization of these simulations and, as enabling technology, the MemCom data management system [1] is deployed, extended and 6S customized. Similar data flow oriented approaches were used in other industrial application oriented projects at CSCS/SCSC [3,4].

Figure 2 shows an exemplary sketch of a typical data flow through 6S, although this figure is largely simplified not containing the complete set of modules. The common data resource brings the advantage of minimising the number of interfaces between modules: for N modules, N two-way interfaces are needed; without a central route of data transfer, N-squared interfaces are needed between N modules. All of the final interdisciplinary demonstrator applications incorporate several modules with specific feedback mechanisms not necessarily visible in the data flow diagram due to the central resource. Common HPCN communication standards such as MPI are regarded as best suited with respect to parallel computation inside the number crunching modules; however the usage of a CORBA bus is under consideration for the coarse grain communication with respect to steering of the execution sequences.

The different forms of 6S are reflected in the layered design of the environment:

- the end-user version will have an advanced graphical user interface with visual programming capabilities
- a language based layer will enable extension and customization
- and the full developer version will provide means to incorporate self-contained modules linked to the CORBA bus.

CSCS/SCSC Involvement

CSCS/SCSC is involved in the tool development for CAD control and repair, the implementation of the geome-

try access service functions for the realisation of the direct interface between the 6S geometry model (an extended BREP representation resulting from CAD repair) and the surface mesh generator of UWS, and the development of grid generation techniques. CSCS/SCSC is also developing interface modules to enable the tightly coupled CFD/CSD analysis by an unstructured fluid simulation code and a structural dynamics code.

While the developments related to preprocessing are evaluated by all end-user partners, the CFD/CSD interface in the present project is directly related to the DASA demonstrator, which targets the aeroelasticity simulation of an aircraft during highly loaded flight manoeuvres. These interfaces will be generic though and exploitable to other CFD/CSD coupling problems.

Conclusion

The JULIUS project is a challenging, high-impact project targeting towards for a standard framework for customization of problem solving environments for engineering applications. It incorporates the complete data flow from standard geometry input data, via mesh generation to standardized data output. The centralized data resource addresses the efficient multi-disciplinary coupling of interdisciplinary applications supported in addition by a CORBA bus for coarse grain communication with respect to application steering.

A whole series of more technical communications is foreseen in upcoming CROSSCUTS issues. The specific development activities of CSCS/SCSC together with its direct partners will appear in one of the very next issues followed by Julius partner's contributions providing a complete picture of the overall project and its future technical outcomes.

A CSCS/SCSC internal JULIUS web-site will be linked to the official Applied Mechanical Engineering (AME) site
http://www.cscs.ch/Official/I2A/AME
which further links to the JULIUS consortium home page.

Acknowledgement

The Julius project is embedded in the ESPRIT IV research programme, the partners acknowledge the support by the CEC. The financial input of the CEC, of the Swiss Government and of the European industrial partners, namely British Aerospace (BAe), Daimler Benz Aerospace (DASA), Dassault Aviation, Engineering Systems International (ESI), Numerical Algorithms Group (NAG) and Stehlin-Merazzi Research (SMR), is appreciated. The technical work programme contains contributions of all Julius partners, i.e., BAe, DASA, Dassault, ESI, IPK, NAG, OUCL, UWS, SMR and CSCS/SCSC. Their responsiveness and active participation lead to the successful preparation of the project.

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[3] R. Gruber, W. Egli, E. Gerteisen, G. Jost, S. Merazzi. Problem-Solving Environments: Towards an Environment for Engineering Applications, SPEEDUP Journal Volume 9/Number 1/July 1995.

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Contacts
John Murphy (john.murphy@src.bae.co.uk)
David Rowse (David.Rowse@src.bae.co.uk)
Luciano Fornasier (luciano.fornasier@lm.otn.dasa.de)
Philippe Thomas (philippe.thomas@dassault-aviation.fr)
Argiris Kamoulakos (ak@esi.fr)
Edgar A. Gerteisen (egerteis@cscs.ch) ■

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Calendar of High-Performance Computing and Related Events

November 1998

7–13 **SC98-High Performance Networking and Computing Conference**
Location: Orlando, Florida (USA)
Contact: SC98, NPACI, UCSD, 10100 Hopkins Drive, La Jolla, CA 92093, USA
Phone: +1 (888) 778 sc98
Fax: +1 (619) 534 8303
URL: http://www.supercomp.org/sc98/

12–13 **JAVADAYS '98**
Location: Frankfurt/Main (Germany)
URL: http://www.sun.de/Homepage/JavaDays98/

15–20 **ASME Forum on Parallel Computing Methods**
Location: Anaheim, CA (USA)
Contact: Dr. Christopher J. Freitas, Southwest Research Inst., 6220 Calebra Rd.
San Antonio, TX 78238-5166, USA
E-mail: cfreitas@swri.edu

16 **Kolloquium zum Geburtstag von Prof. Joerg Waldvogel**
Location: Zurich (Switzerland)
Contact: Gisela Gassmann
Dept. Mathematik, ETHZ, CH-8092, Zurich
E-mail: gassmann@math.ethz.ch, or kraemer@sam.math.ethz.ch

18–20 **50th Anniversary of Applied Mathematics**
Location: Zurich (Switzerland)
E-mail: kraemer@sam.math.ethz.ch
URL: www.sam.math.ethz.ch/reg_d.html

20 **12th Prognose Zirkel Zürich Info Day**
Location: Zurich (Switzerland)
URL: http://www.scsc.ethz.ch/PZZ/

26–27 **CAPTECH98-IFIP Workshop on Modelling and Motion Capture Techniques for Virtual Environments**
Location: Geneva (Switzerland)
E-mail: Christian.Zanardi@cui.unige.ch
URL: http://miralabwww.unige.ch/captech98

December 1998

13–16 **WSC'98-The Winter Simulation Conference**
Location: Washington, DC (USA)
URL: http://www.wintersim.org/index.htm#top

14–16 **PDCN'98-Second IASTED International Conference on Parallel and Distributed Computing and Networks**
Location: Brisbane (Australia)
Contact: Mrs. Pen Harms, IASTED PDCN'98 Secretariat
1811 West Katella Avenue, Suite 101, Anaheim, CA 92804. USA
Phone: +1 (714) 778 3230
Fax: +1 (714) 778 5463
E-mail: iasted@iasted.com
URL: http://www.iasted.com
http://www.cit.gu.edu.au/~hong/pdcn98

16–18 **OPODIS'98-International Conference On Principles Of DIstributed Systems**
Location: Amiens (France)
E-mail: opodis@laria.u-picardie.fr
URL: http://www.laria.u-picardie.fr/OPODIS/page98.html

17–20 **HiPC '98-5th International Conference on High Performance Computing**
Location: Chennai (Madras), (India)
URL: http://www.hipc.org/

January 1999

9–12 **HPCA-5-Fifth International Symposium On High Performance Computer Architecture**
Location: Orlando, FL (USA)
URL: http://www.cse.psu.edu/hpca5/

February 1999

3–5 **PDP 99-7th Euromicro Workshop on Parallel and Distributed Processing**
Location: Funchal (Portugal)
URL: http://www.elet.polimi.it/pdp99/

15–19 **Technologies for Petaflop Computing**
Location: Santa Barbara, CA (USA)
URL: www.cacr.caltech.edu/pflops2/

21–25 **IEEE Frontiers 99 Conference: The 7th Symposium on Frontiers of Massively Parallel Computing**
Location: Annapolis, MD (USA)
URL: http://cesdis.gsfc.nasa.gov/frontiers/front99.html