PDC NEWSLETTER

PDC Conference

In December, PDC traditionally arranges a conference on parallel and high-performance computing. The '96 conference took place at KTH the 16 and 17 of December and the theme this year was "Software for Parallel Computing".

Professor Jack Dongarra from University of Tennessee gave two lectures, a summary of High-Performance Computing Technologies today and a lecture titled "Providing Access to High Performance Computing Technologies". In this speech Professor Dongarra presented the NetSolve project, a numerical library that distributes computations over a network. This can be a local network or an international network.

Dr. Carl Kesselman from University of Southern California presented the Globus Metacomputing Environment. This project develops a.software infrastructure for computations that integrate geographically distributed computational and information resources. PDC is the first European partner to participate in this project.

Some videos showing current research at Carniege Mellon were presented by Professor Raj Reddy. These examples showed some non-traditonal areas for High Performance Computing such as speech recognition, virtual cameras and self driving vehicles. In conjunction with the conference, Professor Reddy also gave a lecture on the UniversalLlibrary Project to librarians from the Stockholm area. The Universal Library is a project to make available all the authored works of mankind on the Internet so that anyone can access this library from any place at any time.

Professor Raj Reddy (left) and Professor Jack Dongarra were two of the international speakers at the PDC Conference.

In This Issue

From the European Centre for Medium-Range Weather Forecasts (ECMWF) in Reading came Professor Geerd Hoffman and presented their Fujitsi VPP 700 system, currently the most powerful computer in Europe according to the TOP500 list.

The GF11 computer project was presented by Dr. Don Weingarten from IBM Watson Research Center. The GF11 is a massively parallel computer specially built and designed for Quantum Chromodynamics (QCD) calculations. By using this computer nonstop for two years, the scientists at IBM have calculated the properties of an elementary particle, called "glueball". This massive calculation, the largest in the history of computing, is the first discovery of a particle by a computer.

During the conference, the KALLSUP computer at KTH were also officially inaugurated. The KALLSUP computer is a Cray J932 owned by a consortium of KTH departments, KALLSUP, but managed by PDC.

EDITORIAL

In the last editorial, we expressed the hope that 1997 would be more focused on a high level of service and new research results, rather than the rapid build-up of infrastructure that signified 1996. Of course, with the constantly evolving technology of high performance computing, there is never a time when the software or hardware infrastructure can be left alone. Nevertheless, there is now more time to support the PDC users and to initiate or strengthen different collaborations. One example is the close working relationship between PDC and the Parallel and Scientific Computing Institute, PSCI.

The science article in this Newsletter comes from PSCI and it covers computational electromagnetics, which is one of PSCIs areas. The institute is a NUTEK Competence Center and it is sponsored in equal parts by NUTEK, Swedish Industry and the university. The funding from HPDR to PDC is solely for academic use. Therefore it is of great help to have PSCI with its industrial emphasis, to handle projects with a large component of industrial research. Computing time at PDC can, for example, be bought by PSCI for individual projects. Research programs with both academic and industrial parts are becoming common due to the funding from European Agencies and the Foundation for Strategic Research.

There are four different research programs in PSCI. Computational electromagnetics was mentioned above and then there are computational fluid dynamics, biocomputing, and parallel tools and implementations. Presently there are ten PhD projects supported by PSCI.

This newsletter also contains a presentation of the Board of PDC and an interview with its chairman PG Hedström. He points out one significant difference between academic and industrial computing centers. The goal and profile of the centers are much better defined in industry. As a national facility PDC must service all academic users and thus should not exclude any field of application. In order to compete on an international level and to be an interesting partner for joint projects, however, it is also very important for PDC to have a clear research profile. PG Hedström is actively working with developing a plan for such a profile.

It is interesting to note that some of the considerations in industry of centralizing the high performance computing resources are the same as those in the academic field. One example is the recent decision of the National Science Foundation in USA to reduce their number of centers from four to two.

This differs from the present picture in Sweden. Right now we are seeing a remarkable increase in the capability of academic high performance computing in many places in Sweden. Recently a Cray T3E has been installed in Linköping, an IBM SP in Umeå and an Origin 2000 at Chalmers. We congratulate these sites to their new systems and we are looking forward to different forms of collaborations.

Björn Engquist

Director

CEM with GFlop/s performance

Ulf Andersson, Gunnar Ledfelt, PSCI, Royal Institute of Techology

This project is a collaboration between Saab Military Aircraft, FOA, SP and NADA at KTH. It is one of the project conducted within the PSCI (Parallel and Scientific Computing Institute) competence center. The goal of this project is to develop methods for numerical simulation of electromagnetic phenomena in complex systems, for instance an aircraft. Electromagnetic fields are governed by the Maxwell equations. For linear, isotropic and nondispersive media they are:

$$\nabla \cdot (\varepsilon \bar{\mathrm{E}}) = 0 \qquad \text{(Gauss)}$$

$$\nabla \cdot (\mu \bar{\mathrm{H}}) = 0 \qquad \text{(Gauss)}$$

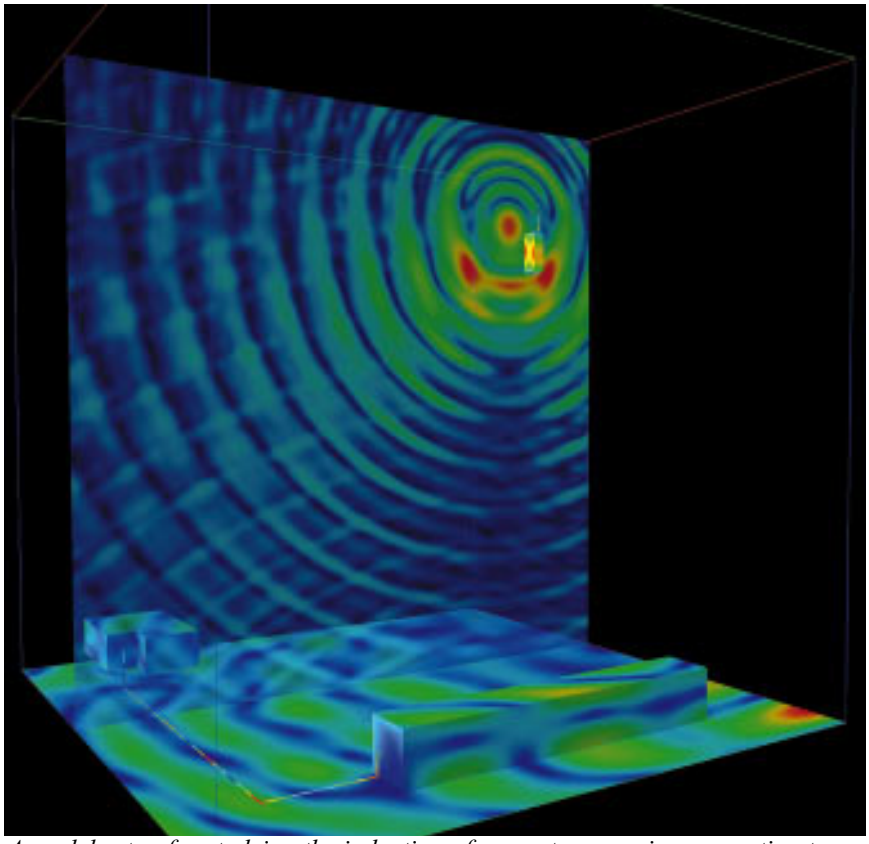
$$\frac{\partial \bar{\mathrm{H}}}{\partial t} = -\frac{1}{\mu} \nabla \times \bar{\mathrm{E}} - \frac{\rho'}{\mu} \bar{\mathrm{H}} \qquad \text{(Faraday)}$$

$$\frac{\partial \bar{\mathrm{E}}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \bar{\mathrm{H}} - \frac{\delta}{\varepsilon} \bar{\mathrm{E}} \qquad \text{(Ampere)}$$

The Maxwell equations are a first order hyperbolic system of PDE:s. They can not be solved analytically except for a few simple geometries, such as spheres and circular cylinders. For more complex structures one has to rely on numerical methods, computational electromagnetics (CEM), and/or experiments.

There is a wide range of applications for CEM. Some of the more important are electromagnetic compatibility (EMC), antenna analysis, cellular phone-human body interaction, microwave ovens and radar cross section (RCS) calculations.

Regarding EMC there are several threats that an aircraft has to be verified against where some examples are lightning, radio and radar fields, electrostatic discharge, fields emitted by electronic equipment and high power directed microwave weapons. All these threats can, if the electronic equipment of the aircraft is not sufficiently protected, disturb or damage the electronic equipment causing EMC problems that would jeopardize flight safety. A well known example is the prohibition of using cellular phones during take off and landing.



A model setup for studying the induction of currents on a wire connecting two electronic devices in the presence of a transmitting cellular phone. The antenna on top of the telephone is driven by a current pulse and the picture shows a snapshot in time of the response. Execution time on the Fujutsi VX/2 at PDC was a few minutes and execution speed almost 900 MFlop/s.

The Yee method

In 1966 a Finite-Difference Time-Domain (FDTD) method for the Maxwell equations was introduced by K. S. Yee. This method uses a leapfrog scheme on staggered Cartesian grids. It explicitly discretizes Ampere's law and Faraday's law and implicitly enforce the two Gauss's law relations.

Calculating the electromagnetic field outside an object usually leads to an open problem, i. e. an infinite computational domain. Therefore, some artificial boundary conditions (ABC) is needed to truncate the computational domain. These boundary conditions must be such that they minimize the reflection of waves trying to leave the computational domain. Incident plane waves can be generated by Huygens surfaces, i.e. by dividing the computational domain into two parts, a total field part surrounded by a scattered field part.

The Yee method has several advantages. It is robust, fast and easy to understand. Furthermore it is possible to achieve the response in a chosen frequency band in one calculation by using a pulse excitation. This can not be achieved with a frequency domain method. On the other hand the Cartesian grid con-

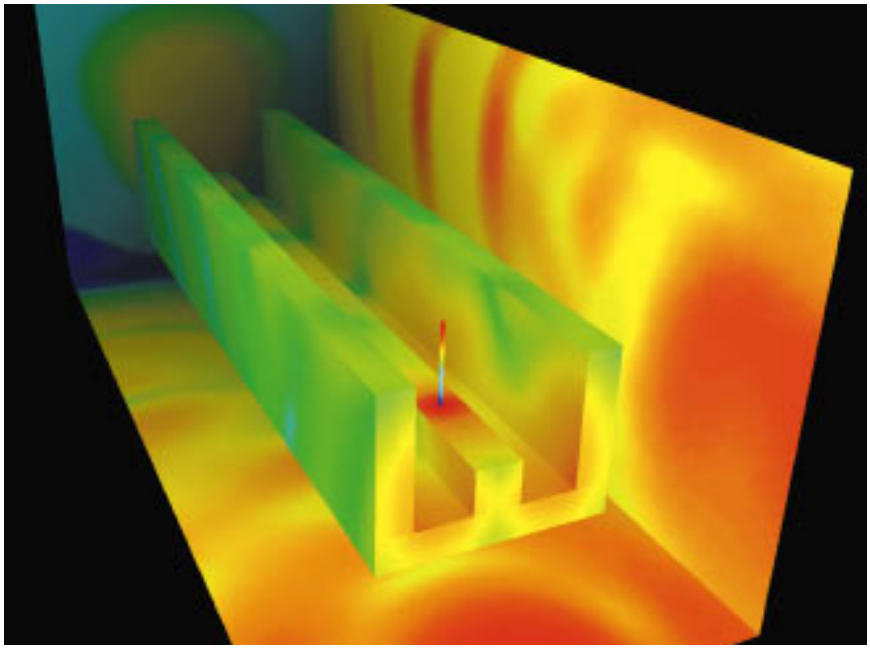
forms badly to the real geometry, thus introducing so called stair stepping errors. Furthermore, it does not exist a general subgridding scheme. This means that structures smaller than the resolution have to be treated by subcell models. In spite of these disadvantages it is foreseen that the Yee method will remain in use for many years. Therefore, the subcell models have to be improved and new subcell models must be developed. Some of the geometric structures in need of (better) subcell models are thin wires, bundled wires, thin layers and thin slots.

Code description

We have implemented the Yee method using Fortran 90. We use the first order Mur boundary condition. The recently introduced Perfectly Matched Layer (PML), is under implementation. PML is regarded as a major breakthrough in electromagnetic modeling. It has been shown to be superior to classical absorbing boundary conditions, such as the Mur boundary condition. Studies of higher order methods are in progress. The code is portable and performs well on the various platforms at PDC. On one IBM SP node the performance is 70 MFlop/s and on one Cray J932 node the perfomance is 100 MFlop/s. On a Fujitsu VX node the code performs extremely well. It is possible to achieve 1.4 GFlop/s. This is more than half of the peak performance (2.2 GFlop/s) of the Fujitsu VX. This performance is however very problem-size dependent. It has been reached on a grid with 2045x59x59 nodes. The two calculations in the figures, with grid sizes of 80x80x200 and 200x200x200, had a performance of about 900 MFlop/s.

In our equations there are twice as many add as there are mult which means that the full arithmetic capacity of the Fujitsu (two add and two mult each clock cycle) can not be used. Therefore, the upper limit of the peak-performance is 1.7 GFlop/s in our application.

Parallelization is under implementation using MPI. Preliminary results on the two node Fujitsu shows a performance of 2.7 GFlop/s for 2045x118x59 nodes. CEM calculations needs a lot of memory. The 2 Gbyte per node at the Fujitsu enables us to make larger simulations than we could perform on a workstation. On 64 thin SP nodes we have reached 3.8 GFlop/s which corresponds to 60 MFlop/s per node and 23% of the peak performance of the SP nodes.



This figure shows, for a distinct time, the solution of an open waveguide problem. An antenna is attached to an E-shaped waveguide and a current pulse is injected into the antenna.

Thin wires

If an electromagnetic problem contains a wire of radius less than the cell size of the FDTD-grid one must use a thin wire model. The purpose of the model is to govern the influence of a wire running through the FDTD-grid without resolving the small wire radius. We have implemented a model that introduces a one-dimensional hyperbolic system of PDE:s describing the current (I) and voltage (V) along the wire. If the wire lies along the z-axis we have,

$$L\frac{\partial I}{\partial t}+\frac{\partial V}{\partial z}=E_z \quad (1)$$

$$C\frac{\partial V}{\partial t}+\frac{\partial I}{\partial z}=0 \quad (2)$$

where L and C are the characteristic inductance and capacitance of the wire.

Equations (1) and (2) are also discretized using a leapfrog scheme on staggered grids. The coupling between the thin wire model and the Yee algorithm is very simple. The right hand side of (1) couples the Yee algorithm to the thin wire model. The coupling from the thin wire model to the Yee algorithm is done by including the current I as a current density term in the right hand side of Ampere's law.

By forcing the current in a wire-segment, the thin wire model can be used for simulating antennas. This procedure has been used in the calculations shown in the figures.

Further information

More information about this project can be found at
http://www.nada.kth.se/~ulfa/CEM.html.

The PDC Board

The members of the PDC Board. From left to right: Jarl Wikberg, Gustav Söderlind, PG Hedström (chairman), Anne-Marie Pilotti, Gunnar von Heijne, and Osvaldo Goscinski. Missing: Lennart Bengtsson, Staffan Ström, Per Dannetun, Håkan Gustafsson, and Jan-Olof Eklundh.

At the last board meeting I had the opportuntiy to ask the chairman, PG Hedström, Corporate Technical Director of Electrolux some questions about how he sees the development of HPCN in Sweden and the role of PDC in the future.

Q: Coming from the industry, what do you see as the main difference between an academic institution as PDC and your company, Electrolux?

A: I think that the talk of differences is sometimes just a prejudice. However, I see one real difference, in the industry we have a very precise goal for each project. PDC is appointed to sustian a national resource. This is a service where the goal isn't as clear as in an industrial project.

Q: Today there is a lot of discussion whether to centralize or decentralize computing resourses. How do you look upon this issue?

A: The mainframe is being reborn again, but only in it's physical sense. Today it seems rational to bring together the resources, there are many advantages: updating software becomes easier, helpdesk functions and education can also benefit from this centralization. From the users point of view, you should not notice the mainframe environment, the users will run their applications on a virtual machine. These virtual machines will be standardized, thus easy to use and maintain.

Sweden or the Nordic countries needs a highly competent center conducting research in these areas. One of the problems to solve is the bandwidth of today's networks. There is also a lot of work that needs to be done with these virtual environments, so that they will offer the same functionallity as today's workstations.

Q: What role will supercomputers and a center like PDC have for industry in the near future?

A: There is today, a lack of knowledge about high-performance computing in industry. The role of PDC is to illustrate which applications that can benefit the industry.

One important task for PDC is to produce research and engineers that have an understanding for HPC. We need the ability to see what problems are suitable for the different levels of hardware and software.

NAG Numerical Libraries

Numerical Algorithms Group (NAG) software has been installed on Strindberg, the IBM SP at PDC. The installed software includes Fortran77 and Fortran90 compilers and tools. Parallel MPI libraries as well as NAGware tools are also a part of the libraries. On-line help is available, instructions can be found on the web page mentioned at the end of this article. The numerical libraries include a vast set of different type of routines. Several of these stem from standard packages like BLAS, LAPACK etc. The parallel libraries are based on BLACS and includes ScaLAPACK routines as well as several routines to aid in data partitioning.

The NAGware suit includes several useful programs which aid the maintenance of Fortran code. In particular, tools are provided for changing a complete code from single to double precision and renaming variables.Pretty printers (source code formatters) and call tree analyzers are also available.

There are also programs for creating uniform declarations which may be used to remove inconsistencies in codes, but also help in the transition from Fortran77 to Fortran90.

More information can be found at:
http://www.pdc.kth.se/compresc/software

Calendar of Events

April

1-5 11th International Parallel Processing Symposium
University of Geneva, Switzerland
http://cuiwww.unige.ch/~ipps97/
email: ipps97@cui.unige.ch

1-5 WRPC '97
Workshop on Randomized Parallel Computing
University of Geneva,Switzerland
http://www.cis.ufl.edu/~raj/cfp97

3-4 **Introduction to Parallel Computing on the IBM SP at PDC**
http://www.pdc.kth.se/training/sp2-intro2.html

8-11 Fractal 97
Fractals in the Natural and Applied Sciences
4th International Multidisciplinary Conference
Denver, Colorado, USA
http://www.kingston.ac.uk/~ap_s412/

9-11 ISADS 97
The Third International Symposium on Autonomous Decentralized Systems
Berlin, Germany
http://www.fokus.gmd.de/ws/isads97/

12-16 Parallel Programming and Java conference
University of Twente, the Netherlands
http://www.rt.el.utwente.nl/wotug20/index.htm

16-18 SPAWC '97
Signal Processing Advances in Wireless Communications
La Villette, Paris, France
http://sig.enst.fr:80/~spawc/

28-30 HPCN Europe '97
Vienna, Austria
http://www.wins.uva.nl/research/HPCN97/
email: hpcn97@wins.uva.nl

May

12-15 JENC8: 8th Joint European Networking Conference
Diversity and Integration: The New European Networking Landscape
Edinburgh, Scotland
http://www.terena.nl/conf/JENC8.html

15-16 **Introduction to Parallel Computing on the IBM SP at PDC**
http://www.pdc.kth.se/training/sp2-intro2.html

19-21 Parallel CFD '97
Implementations and Results Using Parallel Computers
Manchester - England
http://www.dl.ac.uk/TCSC/CompEng/MEETINGS/CFD97/

June

3-4 DSP 97, SCANDINAVIA
Stockholm, Sweden
http://www.dsp-europe.co.uk/scandinavia/index.htm

10-13 PADS'97
11th Workshop on Parallel and Distributed Simulation
Burg Lockenhaus, Austria
http://www.it.kth.se/labs/sim/pads97

18-21 PPoPP 97, SIXTH ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming
Las Vegas, Nevada
http://www.tc.cornell.edu/PPoPP/

22-24 MPPOI'97
Fourth International Conference on Massively Parallel Processing Using Optical Interconnections
Montreal, Canada
http://www.usc.edu/dept/ceng/pinkston/MPPOI97.html

30-July 2
The 1997 International Conference on Parallel and Distributed Processing Techniques and Applications, PDPTA'97
Nevada, USA
http://www.cps.udayton.edu/~pan/pdpta

July

10-12 11th Annual International Conference on High Performance Computing Systems, HPCS'97
Manitoba, Canada
http://www.cs.umanitoba.ca/~hpcs97

14-16 ASAP 97
11th International Conference on Application Specific Systems, Architectures and Processors
Zurich, Switzerland
http://www.tik.ee.ethz.ch/ASAP

14-18 INTERACT97
Sydney, Australia
http://www.acs.org.au/interact97/

August

5-8 HPDC-6
Sixth IEEE International Symposium on High Performance Distributed Computing
Portland, Oregon
http://www.npac.syr.edu/projects/hpdc

18-29 **PDC Summer School 97**
Introduction to HPC.
PDC, KTH, Stockholm
http://www.pdc.kth.se/training/training.html

18-20 SCAI '97
Sixth Scandinavian Conference On Artificial Intelligence
Helsinki, Finland, August 18-20, 1997
http://www.cs.helsinki.fi/events/SCAI97/

26-29 Euro-Par'97
Passau, Bavaria, Germany
http://brahms.fmi.uni-passau.de/cl/europar97/

September

16-19 ParCo97
Parallel Computing Conference
Bonn, Germany
http://www.gmd.de/SCAI/parco97

October

13-16 9th IASTED International Conference on Parallel and Distributed Computing and Systems.
Georgetown University, Washington, D.C., USA.
http://www.mcs.newpaltz.edu/pdcs97

November

5-8, HiPer' 97 High Performance Computing on Hewlett-Packard Systems
Krakow, Poland
http://www.cyf-kr.edu.pl/hiper97/

Introduction to Parallel Computing on the IBM SP at PDC

This course gives an introduction in using and writing parallel programs on the IBM SP computer at PDC. The course includes a general overview of parallel computing, compilers and software development tools on the SP and message-passing programming by MPI.

The course spans two days with lectures in the mornings and excercises in the afternoons.The course will be given at three occasions during the spring: 6-7 March, 3-4 April, and 15-16 May. For more information and to sign up for the course see our web page:

http://www.pdc.kth.se/training/sp2-intro2.html

Apply for Computer Time at PDC now

The next deadline for applying is May the 5:th, so send in your applications before this date. We have made some small changes to the application forms. The new application form can be found at:
http://www.pdc.kth.se/support/accounts.html
Applications can be submitted at any time. However, meetings for evaluation of applications are planned to May, September, and November.

PDC Summer School 97

An intensive two week summer school course "Introduction to HPC" will be arranged August 18-29 on the KTH campus. The course will carry five academic credits. For full academic credit the student must complete a post-course project. Industrial participation is most welcome, and potential industrial users should contact PDC directly (see back cover for details). The number of seats is limited. Grants to cover the costs for a number of academic participants will be awarded based on application.

A block of hotel rooms near KTH will be available for a reduced charge.

A number of topics will be covered in overview lectures given by international experts and in in-depth technical lectures followed by hands-on computer lab sessions.

The areas covered at the course will span the following topics:

- The PDC Computing Environment
- HPC Programming and Message Passing Libraries
- Modern Computer Architectures
- Parallel Algorithms
- Computer Visualization
- Efficient Programming
- Applied Software and Mass Storage

For application forms contact PDC (see back cover) or see our web page: http://www.pdc.kth.se/training/training.html. More information about the summer school can also be found at this web page.

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PDC NEWSLETTER

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The center operates leading-edge, high-performance computers as easily accessible national resources. These resources are primarily available for Swedish academic research and education.

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