PDC NEWSLETTER

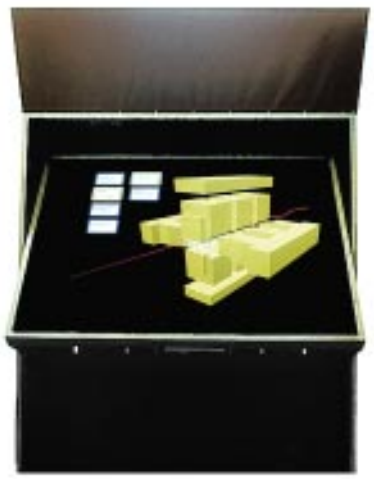
Positive evaluation of PDC

During October 23-24 PDC was visited by an evaluation committee appointed by the Swedish Council for High-Performance Computing, HPDR. Their task was to provide HPDR with recommendations upon which the council can base a decision regarding future funding of PDC. The committee had the following members: Professor Jan S Nilsson, Knut and Alice Wallenberg's Foundation, Professor Risto Nieminen, CSC, Finland, and Professor Odd Gropen, Dept. of Chemistry, University of Tromsø, Norway. The criteria being evaluated were the service level of PDC, user satisfaction, the hardware and software configuration, and the plans for the future of PDC.

After a thorough examination, the committee presented a report. In this report the committee states that the PDC system has reached and in some cases exceeded the level that can be expected from a national facility. A user survey provided by HPDR shows that many users regard PDC as an enabling factor in their research. The staff is praised for its efforts and friendliness, and the educational efforts are appreciated by our users.

The overall impression is very positive, the report summarizes "..the committee concludes that PDC has in all respects met the criteria set out in the evaluation instruction".

This positive report and the following decision by HPDR will provide funding for PDC in the next three years, enabling us to reach the outlined 250 GFlop/s peak performance capacity in the next few years.



The ImmersaDesk showing a demonstration application.

In This Issue

Visualization lab at PDC

Recently PDC purchased an ImmersaDesk from Pyramid Systems. The ImmersaDesk is a 3D vizualisation tool based on a stereoscopic projectction system with a 45 degree angled screen. This allows the user to look down and forward, experiencing both birds-eye and elevation views. The size of the system is similar to that of a drafting table, the heigt being approximately 2.6 m and the width a little less than 1.8 m.

In order to see the 3D images you need a pair of glasses, we use Crytstal Eyes, which uses liquid crystal lenses to open and close alternately in front of your left and right eye.The projection is controlled by a tracking system with six degrees of freedom. The tracking system follows your movements, via a sensor on the glasses and a free-moving joystick. The glasses communicates with the ImmersaDesk via IR.

The projected imagery is created by a Silicon Graphics Onyx.

This is technique has not yet been fully explored by us, but the possibilities are very exciting. There are applications to be found in many different scientific areas such as engineering, medicine, molecular chemistry, anatomy, geophysics, neuroscience and architecture to mention some. The ImmersaDesk has a great potential to make your data come alive and, of course, also be used directly for research in virtual reality..

A PC-based video editing facility has also been acquired.

EDITORIAL

The year 1996, in which PDC opened as a HPDR facility is coming to a close. It has clearly been the most important year for PDC and thus also important for its users. PDC has operated as a center following the HPDR rules since March and it was evaluated during October by an expert committee appointed by HPDR.

The report from the evaluation committee was both detailed and supportive. Here is a quote "The overall impression of the committee was very positive and given the short build-up period PDC has managed remarkably well in reaching the desired level of service."

Since the last newsletter the upgrade of the SP2 Strindberg to 110 processors has been completed and and is in full production. Strindberg is now capable of 29 Gflops peak and has 20 GB of memory. PDC has also obtained an ImmersaDesk for its visualization lab, see the article on the front page for details.

As a result of the established reputation of PDC follows interesting joint projects with different vendors. SGI/CRAY will place an 8 processor ONYX2 at PDC for half a year. The PDC users can access the ONYX2 for visualization projects or for general purpose computing. We encourage our users to take the opportunity to test this new computer which replaces the Powerchallenge and has a very promising architecture.

The European Commission has initiated a program for linking centers in high performance computing. The centers in this network are called Technology Transfer Nodes (TTNs) and they should reach out to industry and promote modern techniques in high performance computing. PDC was recently selected as a regional TTN for Sweden and Norway. There are about twenty TTNs and it is an honor to be part of a network which includes many of the leading scientific computing centers in Europe. The increased contacts with other centers should benefit the PDC users and should also initiate new industrial cooperation.

It has been popular to speculate in the future of super computing. Will its importance increase or decay? It seems that the improved communication and the capability of parallel computing point to increased importance at the present time. One sign of this could be seen at the recent super computing conference in Pittsburgh. There was little in the way of new hardware but the ASCI project from the US Department of Energy points to a bright future.The acronym ASCI stands for Accelerated Strategic Computing Initiative. The nuclear test ban treaty means that all experiments must be replaced by very large scale computer simulations in order to maintain the nuclear stock pile. Already in two years the first computers should reach sustained tera flop performance. Hopefully this gigantic effort will have peaceful spin-offs.

The year 1996 required a rapid development of the infrastructure at PDC. We are now looking forward to 1997 and we hope to see many examples of excellent research projects resulting from this infrastructure. It will be exciting to follow the outcome of the early projects.

Best wishes for the holidays and happy computing in 1997.

Björn Engquist

Director

Molecular Dynamic Study of Melting Earth's Materials

Anatoly B. Belonishko, Institute of Earth Sciences, Uppsala University

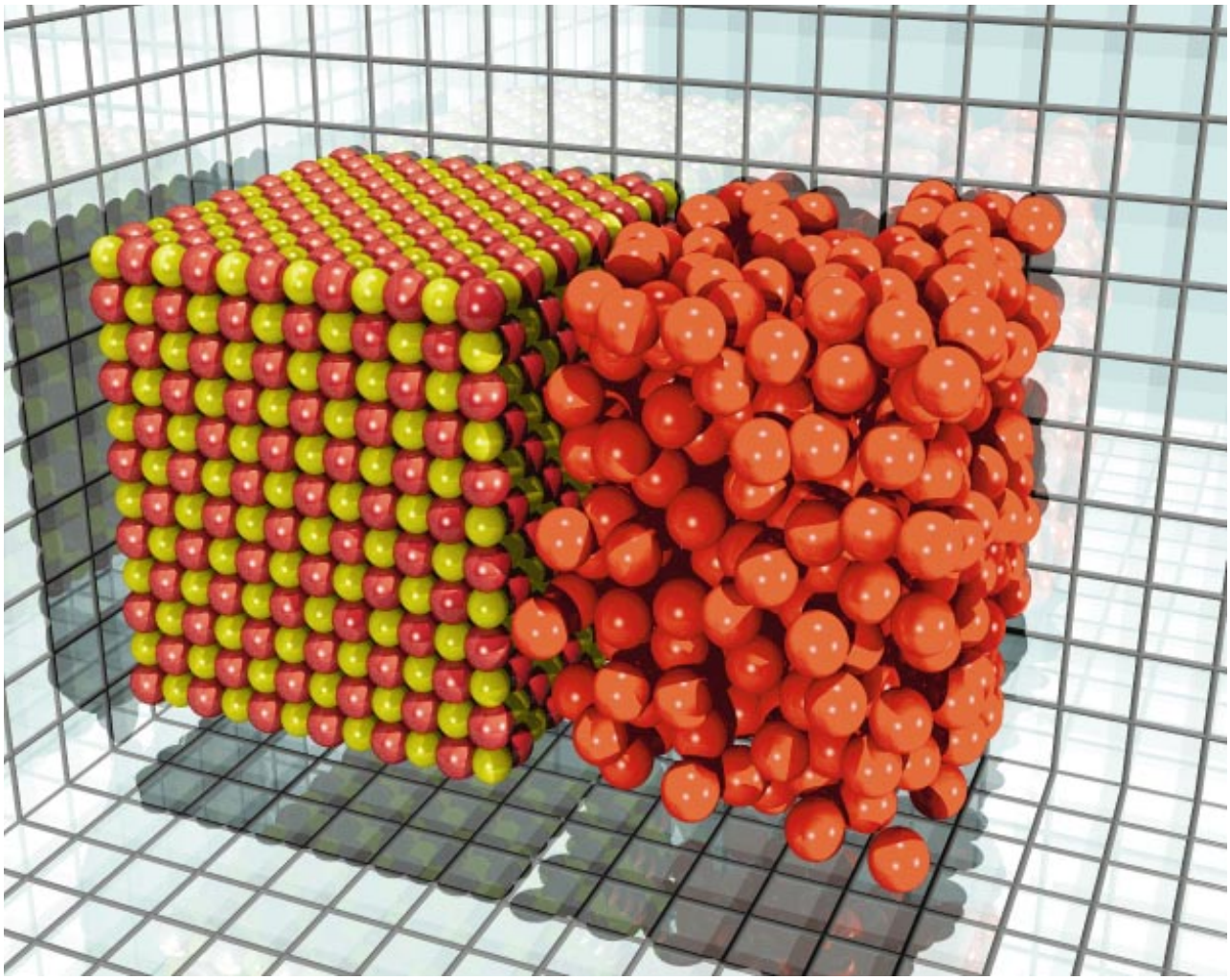


Figure 1
A perfect MgO crystal (smaller spheres) being pressurized by Argon (larger red spheres).

Our knowledge of the Earth's composition comes mainly from the cosmic abundances of the elements. Based on these data in combination with phase equilibria in such materials and seismic data the Earth is viewed as being composed mostly of silica and a $MgSiO_3$-perovskite mantle, and an iron liquid outer and solid inner core. The range of pressures relevant to studies of the Earth materials is from 1 to more than 3.5 million atmospheres. Naturally, experimental studies are extremely difficult at such a high pressure, especially in combination with high temperature. The problem of melting is of particular importance for the Earth science, because there are a number of factors which critically dependent on melting temperatures. Theoretical studies allow us to get insight into the mechanism of melting at very high pressures and provide very reasonable estimates of melting temperatures.

We have studied the melting of SiO_2 (stishovite and quartz), $MgSiO_3$ (perovskite), NaCl (B1 and B2 phases - as a test), MgOFe (bcc, fcc, and hcp phases) using the molecular dynamic (MD) method and the Strindberg SP computer at PDC. Apart from the problem of description of interatomic interaction, the simulation of melting requires adequate choice of simulation technique because of the well known phenomenon of overheating in MD simulation of melting. To avoid overheating, the so called two-phase simulation have been carried out. An initial computational cell containting 2048 atoms of iron was composed of a solid and a liquid portion put together as shown in Figure 2(a). Starting from such an initial configuration simulations have been performed at a given temperature and pressure. If the sample became a crystal (Figure 2(b)) then in the next run temperature was increased and simulations were repea-

ted raising temperature until the sample became molten (Figure 2(c)). In such a way it was possible to determine an exact position of the melting temperature at a given pressure. The use of parallel computers are crucial in such simulations, because the choice of temperature in the next run depends on the results of the previous one. Therefore, the runs can not be performed independently and require a fast computer. The use of the two-phase simulation method was demonstrated to be equivalent to the method of free energy calculations and allows us to calculate melting temperatures of modeled systems very precisely.

Because of significant experimental problems of ultra-high pressure-temperature experiments, computer simulation becomes equal copartner of experimental studies. For example, MD computer simulations of experiments employing diamond anvil cell technique with laser heating have allowed to reveal the importance of thermal stress. A typical computational cell in those studies is shown in Figure 1. A perfect MgO crystal was pressurized by Argon. However, different pressures were applied to different faces of the MgO crystal. When the difference in pressure reaches a critical value, recrystallization is observed. This has allowed to solve the experimental problem of systematically too low melting temperatures when the diamond anvil cell technique with laser heating is employed.

The size and time scale of simulation is out of reach of serial computers. Without distributed calculations these studies will hardly be feasible.

Among the applications employed two might be of use to those interested in running molecular dynamic (MD) simulation on parallel platforms. These are the MD software packages Moldy (http://www.earth.ox.ac.uk/~keith/moldy.html) and DL_POLY (http://gserv1.dl.ac.uk/CCP/CCP5/dl_poly.html). Both are available to academic users free of charge under agreement on certain conditions. The attractive feature of both programs is that the source code is provided which can be easily modified. Moldy is written in C and DL_POLY in FORTRAN. The packages are well documented and easy to use.

The use of parallel computers are crucial in such simulations...

Moldy is a computer program for performing MD simulations of condensed matter. It can handle any assembly of rigid polyatomic molecules, atoms or ions and any mixture thereof. It uses the "link-cell" method to calculate short-range forces and the Ewald sum technique to handle long-range electrostatic forces. Simulations can be performed in practically any ensemble using, among other possibilities, Nose-Hoover thermostat and Parrinello and Rahman constant-stress methods. DL_POLY package also includes possibility to simulate macromolecules and is capable to handle 3-body forces and embedded-atom potentials of Sutton-Chen type. This potential provides opportunity to simulate metalsin which volume-dependent energy term is substantial.

The Moldy homepage contains benchmark results for running Moldy on sixty different computer platforms. The benchmark is for the version 2.0 and the current available version is 2.11. The timing results are obtained calculating system of 64 TIPS2 molecules. A comparison of the current version (2.11) of Moldy shows that it runs with almost the same speed on IBM SP2 (1 processor) as the version 2.0 on Cray X-MP. The scaling performance is about 70% with 16 processors when simulating a system of 64 water molecules and close to 90% for a larger system. This is better than scaling performance on Cray Y-MP. The run for 4000 time steps on 16 processors of IBM SP2 only takes 41 seconds. It is worth to mention that about 15-20 years ago such simulation was rather serious computational problem which required a few hours of computing time on IBM 360 mainframe.

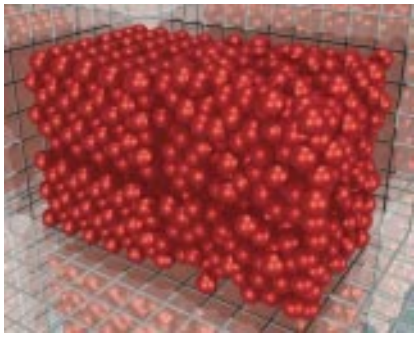


Figure 2(a)
Initial state, a solid and a liquid portion.

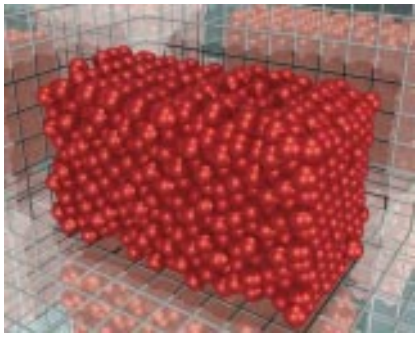


Figure 2(b)
Solid iron crystal.

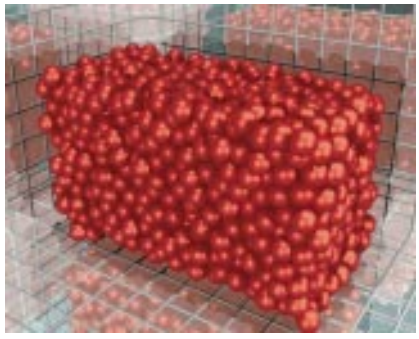


Figure 2(c)
Calculated molten configuration.

New Fujitsu VX/2

Selma, a Fujitsu VX/2, is the latest computer at PDC. We continue to name computers after famous Swedish authors and Selma is named after Selma Lagerlöf, the 1909 Nobel Laureate in literature. Selma was installed during the summer and has been tested by selected users at PDC since then. We would now like to announce Selma as available for the users at PDC.

The Fujitsu VX/2 is a distributed memory vector computer. The VX is the smallestsystem in the VPP series with the VPP-300 and VPP-700 systems at the high end. These computers are implemented in mass-market technologies, CMOS VLSI and DRAM memories, and offer very competetive price-performance.

The Fujitsu VPP architecture is alreay widespread in Japanese academia and industry. It is quickly becoming widespread in Europe. For example, the European weather center in Reading, ECMWF, has invested in a very large VPP system.

The number 2 in the model Fujitsu VX/2, means that Selma is equipped with two processing elements. The processors have vector architecture and achieve 2.2 GFlop/s and have 2 GByte of memory each. The processors are connected through a crossbars switch with 570 MByte/s transfer rate in each direction. Real applicaton achieve about 400 MByte/s in each direction. Selma has 28 GByte of disk.

Selma has shown to be very fast at vector calculations. In an application of computational electromagnetics Ulf Andersson, Gunnar Ledfelt, Anders Ålund, and Per Hammarlund from KTH have achieved about 1.3 GFlop sustained on one processor. On certain ABAQUS single-processors job the Fujitsu VPP outperforms the CRAY T90. For suitable vectorized code it is possible to reach 50-70% of the peak performance.

The OS, UXP/V is based on the UNIX System V release 4, and the machine behaves as a UNIX workstation. Batch processing is managed by NQS. The most mature programming environment is based on Fujitsu's Fortran90 compiler. C compilers are also available. The PVM message passing environment is available and MPI will be available soon.

The new Fujitsu VX/2 at PDC.

See http://www.pdc.kth.se/compresc/machines/selma.html or have a look at the Fujitsi's super computer group homepage at: http://www.fujitsu.com/FAI/SCG/scg_dot/1-scg-front.htm for more information about Selma.

PDC appointed as TTN

PDC has been selected as a Technology Transfer Node (TTN) in a programme initiated by the European Commission. By becoming a TTN we join a European Network with more than 20 members such as CSC in Finland, UNI-C in Denmark, University of Edingburgh and PAC in the UK, and GMD in Germany.

The aim of a TTN is to raise awareness of High Performance Computing & Networking (HPCN) in industry, especially small and medium-sized companies. A TTN helps companies to assess potential gains of HPCN use, demonstrates the abilities of current HPCN technology, and encourages companies to use HPCN.

Demonstration includes showing how existing applications would benefit business by the use of HPCN technology. This can be acheived through porting, or migrating in a wide area network based environment. A demonstration can also be field tests, where you show the viability of new prototypes to be converted in to operational prototypes or new products.

As a TTN PDC will formulate actions together with industry to develop the use of HPCN at the industry end-user. Cost for this action will be supported by the commission up to 50% for industry and to 100% for PDC.

The activities will cover a broad range of user organisations, both in terms of industrial sector and in terms of company type.

Areas in focus for the PDC-TTN will be computational electromagnetics, computational fluid dynamics, visualization, and computer security.

Calendar of Events

December

2-5 The 1996 Asian Computing Science Conference
Singapore
http://www.iscs.nus.sg/~asian96

3-4 Workshop on Scientific Visualization
PDC
email:johani@pdc.kth.se

3-6 Gaussian Workshop
Liege, Belgium
email: info@gaussian.com

11 Workshop on Computational Electromagnetics
PDC
email:per@pdc.kth.se

16-17 Annual PDC Conference
Software for Parallel Computing
http://www.pdc.kth.se/news/events/conference96/
email: gert@pdc.kth.se

January 97

7-8 Computational Differential Equation Circus
The Department of Informatics,
University of Oslo
http://www.imf.unit.no/cde-circus/

8-March 7
Virtual Workshop
Parallel Programming with Message-Passing Libraries
Cornell Theory Center
http://www.tc.cornell.edu/Edu/VW/

22-24 5th EUROMICRO Workshop on Parallel and Distributed Processing
London, United Kingdom
http://www.par.univie.ac.at/PDP97/
email: pdp97@par.univie.ac.at

February 97

1-5 HPCA3, Third International Symposium on High-Performance Computer Architecture
San Antonio, Texas
http://www.ece.ncsu.edu/hpca3/

10-14 The Fifth International Conference in Central Europe on Computer Graphics and Visualization'97
University of West Bohemia, Czech Republic
http://yoyo1.zcu.cz/~skala/wscg97.html
email: WSCG97@kiv.zcu.cz

24-26 First Annual High Performance Fortran User Group Meeting
Sante Fe, New Mexico
http://www.lanl.gov/HPF

March 97

13 SIAM Short Course on Performance Programming for Scientific Computation

14-17 Eighth SIAM Conference on Parallell Processing for Scientific Computation.
Minneapolis, Minnesota
http://www.siam.org/meetings/pp97/pp97home.htm

17-21 European Research Seminar in Distributed Systems
Zinal, Switzerland
http://lsewww.epfl.ch/conferences/ersads.html

April 97

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

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/

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

May 97

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

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

June 97

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

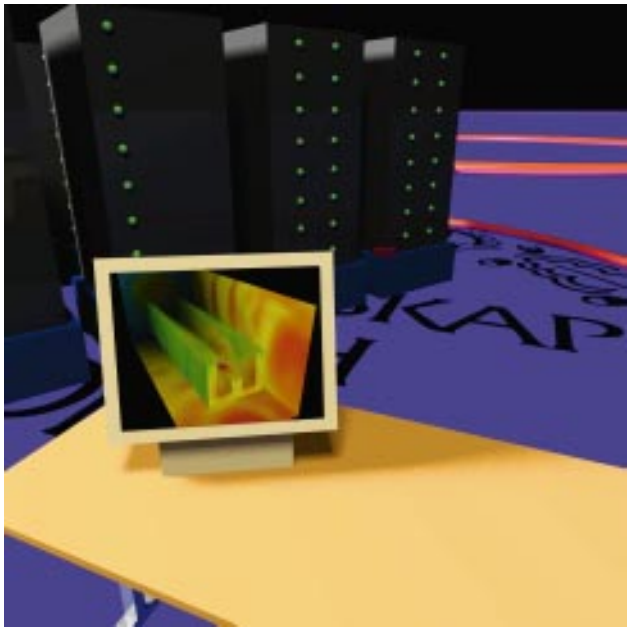
25-27 Fractals In Engineering
Arcachon, France
http://www-syntim.inria.fr/fractales/Confs/FracEng.html
email: FE97@inria.fr

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 97

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

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



Progress Report 1994 - 1996

The new Progress Report from PDC is now available. The report presents the research activities done here at PDC by our users. The research covers many areas such as chemistry, physics, biology, computational electromagnetics, computational fluid dynamics, and geophysics.

Among the content of the report you'll find a different version of the article about melting Earth's materials on page 3 and you may also find a more elaborate version of the article "An integratal direct distributed-data, parallel MP2 algorithm" presented in the last Newsletter.

The week of the 9-graders

During the week from the 4:th to the 8:th of November KTH organized "The week of the 9-graders". During this week schools from all over the county of Stockholm came to visit KTH.

More than two hundred pupils visited PDC during this week for a short introduction to super computers. We offered a brief presentation of PDC and a short example of scientific computing. They also had a chance to discuss which stream to follow in the upper secondary school, in Swedish called the "gymnasium". The visit ended with a peek at the computers here at PDC. We are always glad to welcome visitors.

B

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Porto
Betalt

PDC Newsletter

Published quarterly by the Center for Parallel Computers at KTH.

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

PDC receives funding from the Swedish Council for High-Performance Computing, HPDR and KTH.

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ISSN 1401-9671

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