PDC Newsletter

No 2 - 2004

Photo: Harald Barth

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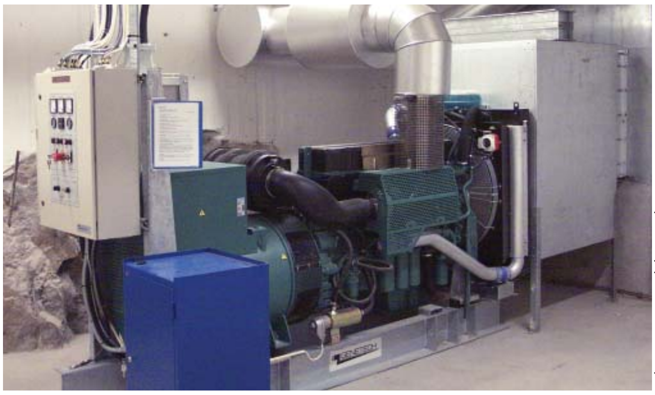

Photo: Harald Barth

Fig 1. Bottles of inert gas for fire extinguishing

Fig 2. Diesel engine and power generator

PDC in New Premises

Gert Svensson, PDC

In the beginning of 2004, PDC moved to newly renovated premises at Teknikringen 14, not far from the previous location in the KTH main building. The relocation of the computer equipment was especially demanding, because we tried to minimize the downtime of each individual system for the benefit of our users.

One important reason for the relocation was that the space for computer equipment had become too small. The old computer rooms had a total area of about 110 m^2 while the current two rooms are 240 m^2 and 32 m^2 respectively. The smaller room has a more fireproof structure and houses the tape robot.

A further important reason was to locate PDC and the KTH Network Operation Center (KTHNOC) in the same building, because the operational aspects of the two units are similar. PDC is also neighboring CVAP (Computational Vision and Active Perception Laboratory) and CAS (Centre for Autonomous Systems).

Improved facilities for computer operation

PDC has a high demand for reliable computer operation; this is even more important for KTHNOC, which should be able to operate without external electrical power and cooling for indefinite amounts of time. To achieve this, KTHNOC uses its own diesel engine driving a power generator. This unit together with other support equipment is located in the building basement. By tapping into this power unit, PDC can operate all servers and other critical computer and cooling equipment without external power. Because of the expense of emergency power equipment capable of indefinite operation, the current equipment is not designed to support all computational clusters at PDC. But, if this need should arise there is space available for a second power unit. ...continued on page 3

Lennart Johnsson
Director of PDC

In This Issue:

PDC Newsletter No 1 - 2004

Published by PDC at KTH.

PDC operates leading-edge, high-performance computing systems as easily accessible national resources and carries out research in soft-ware and tools for use and administration of such systems. The hardware resources and the costs of their operations are largely covered by funding from the Swedish Research Council and KTH. The research is funded from a variety of sources with the majority of research funds coming from the European Commission.

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Leader

This issue is focused on our new facilities for equipment and two exciting research projects. PDC is both a service center and a center of excellence. The service center component of PDC provides user support and operates and maintains high-performance computing and storage systems for the Swedish academic community on behalf of SNIC, the Swedish National Infrastructure for Computing, funded by the Swedish Research Council; PDC also provides support for research groups with sufficient needs and funds to acquire their own resources, such as SBC, the Stockholm Bioinformatics Center, and the KTH Kallsup consortium. The research is focused on challenges related to high-performance and large-scale computation and data management, such as Grid technologies, performance engineering, visualization, and management of scalable computer and storage systems.

Moore's Law, which shows computing capability increasing exponentially over time while cost remains constant, is well known. Increased capability has also increased the power density significantly. Heat removal has become a design issue at all levels, from the chip level to computer room design and system placement, the latter being major concerns for PDC. From the Intel i386 to the Pentium IV, power density has increased from about 1 W/cm^2 to 30-40 W/cm^2. For comparison, a typical hot plate operates at about 10 W/cm^2. Today, power ratings for dual processor nodes in clusters may be as high as 600 W. System vendors now use sophisticated cooling techniques to handle heat loads and enable the tight packaging used in blade technology. This development has resulted in power requirements of about 10 kVA per rack, with extreme packing resulting in requirements in excess of 20 kVA per rack. These power densities and associated heat loads represent significant challenges in placement of racks and computer room design to avoid hot-spots. An example of high power demands is the well-publicized Earth Simulator that is housed in its own building with a computer room floor of 3250 m^2, and its own 15 MVA power plant.

Our new facilities represent a significant investment of KTH and NADA to accommodate the growing needs for space, power, and cooling for computing and storage systems managed by PDC, currently close to 600 nodes with a capacity of about three TFlops. About 60% of the nodes and 55% of the capacity are operated for SBC, and the majority of the remaining systems are operated for SNIC. With procurements currently under way for SNIC, we expect to double the computational capabilities under PDC management. This very exciting development would not have been possible in our old facilities.

We welcome our users and other readers of this newsletter to visit us at our new facilities.

...continued form page 1. All computer equipment at PDC and KTHNOC is protected by UPS (Uninterruptible Power Supplies) systems. They eliminate power quality problems and protect from short power outages by using large batteries. For equipment covered by the power generator, the UPS system only needs to supply power from the start of a power failure until the diesel starts, which normally takes less than a minute. The UPS system for the computational clusters is capable of supplying 230 kW of power during 30 minutes, sufficient to operate more than 6 TFlops of state-of-the-art computing equipment and associated storage systems. At the moment the equipment managed by PDC requires about 130 kW of power. However, with the acquisition of new equipment under way the capability of the current UPS system will be exceeded and not all equipment will be covered for 30 minutes of operation.

Photo: Harald Barth

Excavating the basement for more space.

This large consumption of electricity produces a substantial amount of heat. To be environmentally friendly, PDC uses district cooling from Fortum, the main energy supplier in Stockholm. Most cooling systems are fairly unreliable, because they include many moving parts. To protect against failure in the cooling units, we use one spare cooling unit in each room. To protect from failure in the district cooling system we have an additional circuit with ordinary tap water.

The value of the PDC computers is substantial, and the value of the stored data is even higher. To protect the computers and data from fire from the outside, the walls of the computer room are more fireproof than normal walls. To protect from fires starting in the electronics or power supplies inside the computer room, we have installed automatic fire detection and extinguishing systems based on inert gases, which are harmless to people.

To supervise all the support units, a Web-based control system is installed, which displays the status and most interesting parameters in a Web hierarchy. The staff is alerted to any problem by email or SMS, or in catastrophic situations also by flashing lights.

In total PDC now has the most modern and reliable environment for computers, which also makes it possible for PDC to continue to grow in the future.

The Architect’s View

Bo Ericson, A&P Arkitektkontor AB.

PDC’s new premises were originally designed by Professor Gunnar Henriksson at KTH and completed in 1962 under the name “Ny Fysik”. One of his former students, Bo Ericson of Ahrbom & Partner, was appointed to lead the renovation of the building. He describes his task in the following article.

Photo: Harald Barth

The building consists of a high-rise section of 7 stories with the main entrance at level 2. The landlord Akademiska Hus provided a brief to improve the spatial and technical facilities for their tenants PDC, KTHNOC, CVAP and CAS. In addition there was a requirement for a new communal space for teaching. The brick and concrete construction of the building presented serious challenges and limited the scope for alteration.

The high-performance computers managed by PDC have been located in the old workshop, a beautiful spacious room on the ground floor of the lower section, which benefits from a lot of daylight and could be suitable for an art exhibition. Located above this server hall are computer terminal rooms for students working on assignments and projects. Here 250 students can find a computer within one of six distinct spaces delineated by structural concrete walls. To assist with orientation, each space is named after characters in Tolkien’s *Lord of the Rings.* Because the dividing concrete walls couldn’t be reconfigured, small holes were created at regular intervals, and mirrors were installed along the wall between each opening to create interesting perspectives; this links the spaces visually and enlivens the environment for the students. The idea came from a bar in London in 1972!

Photo: Harald Barth

Photo: Harald Barth

All office space for the scientists and teachers has been located in the high-rise section of the building. Each of the three tenants occupies two floors, which are connected with narrow staircases. To bring daylight and a sense of openness to the corridor areas, sliding glass panel doors and glazed slits were installed to all office rooms. Immediately adjacent to PDC's entrance, it was possible to remove a section of the corridor wall, where a curved section of casing taken from the old 'supercomputer' acts as an informal reception desk, hiding PDC's post and photocopy facilities.

One of the biggest challenges of the project was to install all the technical equipment within the limited space of the cellar. A lot of dynamite was required to create new spaces for the diesel engines and fans that ventilate and cool the building. The entire project was executed on a tight time schedule arising from a series of departments within the campus moving location at the same time.

The renovation also upgraded the handicap facilities in compliance with current building legislation. A new staircase and ramp leading up to the main entrance from a small park, which will contain spectacular art pieces provided by Statens Konstråd, was constructed.

Photo: Harald Barth

Calendar

- July 18-30, 2004, Naples, Italy: Second International Grid Summer School 2004; http://www.dma.unina.it/~murli/GridSummerSchool2004
- July 24-28, 2004, Jyväskylä Finland: European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2004); http://www.mit.jyu.fi/eccomas2004
- July 26-30, 2004, University Of Leuven Belgium: Congress in Belgium on Computational and Applied Mathematics; http://www.cs.kuleuven.ac.be/conference/iccam2004/iccam.htm
- July 26-30, 2004, Portland, OR, USA: O'Reilly Open Source Convention; http://conferences.oreillynet.com
- July 27-29, 2004, Tysons Corner, VA, USA: Cluster Symposium 2004; http://www.arl.hpc.mil/Clusters2004/index.html
- August 3-5, 2004, San Francisco, CA, USA: LinuxWorld Conference & Expo; http://www.linuxworldexpo.com
- August 8-12, 2004, Los Angeles, CA, USA: SIGGRAPH 2004 – 31st International Conf. on Computer Graphics; http://www.siggraph.org/s2004
- August 15-18, 2004, Montreal, Quebec, Canada: ICPP-04, The 2004 International Conference on Parallell Processing; http://www.ecn.purdue.edu/icpp2004
- August 16-17, 2004, Stockholm, Sweden: PDC Summer School: Introduction to High-Performance Computing; http://www.pdc.kth.se/training/summerschool
- August 22, 2004, Seattle, WA, USA: BIOKDD04: 4th ACM SIGKDD Workshop on Data Mining in Bioinformatics; http://www.cs.rpi.edu/~zaki/BIOKDD04
- August 31 - September 3, 2004, Pisa, Italy: Euro-Par 2004; http://www.di.unipi.it/europar04
- September 6-10, 2004, Marne la Vallée, France: EUROSIM04 - Fifth Conference on Modelling and Simulation; http://www.esiee.fr/~eurosim4
- September 7-10, 2004, Dresden, Germany: PARELEC 2004, The Fourth International Conference on Parallel Computing in Electrical Engineering; http://www.parelec.org
- September 10-14, 2004, Chalkis, Greece: International Conference of Numerical Analysis and Applied Mathematics 2004 (ICNAAM 2004); http://www.uop.gr/~icnaam
- September 15-17, 2004, San Francisco, CA, USA: PDCS-2004, 17th International Conference ond Parallel and Distributed Computing; http://multimedia.ece.uic.edu/pdcs2004
- September 19-22, 2004, Budapest, Hungary: 11th European PVMMPI Users' Group Meeting; http://www.lpds.sztaki.hu/pvmmpi
- September 20-23, 2004, San Diego, CA, USA: Cluster 2004: The 2004 IEEE International Conference on Cluster Computing; http://grail.sdsc.edu/cluster2004
- September 27 - October 1, 2004, Albuquerque, NM, USA: Linux Clusters Institute; http://www.linuxclustersinstitute.org
- September 29 - October 3, 2004, Antibes Juan-les-Pins, France: PACT'04, 13th International Conference on Parallel Architectures and Compilation Techniques; http://www.pactconf.org
- October 4-6, 2004, Moscow Russia: Parallel Computations and Control Problems PACO '2004, II International Conference; http://paco.sicpro.org
- October 18-20, 2004, Wuhan, China: NPC2004,IFIP International Conference on Network and Parallel Computing; http://grid.hust.edu.cn/npc04
- October 18-20, 2004, Linköping, Sweden: 5th Workshop on Linux Clusters for Super Computing (LCSC); http://www.nsc.liu.se/lcsc
- October 21, 2004, Wuhan, China: GCC 2004 - Third International Conference on Grid and Cooperative Computing; http://grid.hust.edu.cn/gcc2004

PDC Network Infrastructure

Harald Barth, PDC

Everyone connecting to PDC's computing resources uses PDC's internal network and PDC's connection to the Internet. In fact, PDC's internal network is "the Internet" as much as every other part of the Internet, so I'll just use "the Net" for short.

The Net is divided into Autonomous Systems (AS), each one forming an administrative unit on its own. Examples for ASes are Sunet, Telia, Geant, and PDC. An AS has network connections to two or more other ASes, in PDC's case to KTH and Sunet. For research and demonstration purposes, now and then PDC has used connections to other ASes farther away, for example to Startap in Chicago. Between ASes, the Border Gateway Protocol (BGP) is used to exchange information where different IP networks are located on the Net. By advertising IP networks to its neighbors and blocking such advertisements, the different ASes control the flow of IP packets throughout the Net. For example, packets are allowed to transit freely from PDC through KTH to Sunet and from KTH through PDC to Sunet. On the other hand, transit from one commercial provider to another through Sunet is prohibited.

At PDC, two routers – Extreme Networks "Black Diamond" routing switches – form a redundant pair that exchange BGP information with KTH's and Sunet's counterparts. All of PDC's connections to the outside are made with Gigabit Ethernet over fiber. On the other side, Cisco 10720 access routers and Cisco 5500 connect to Sunet's and KTH's infrastructures. KTH's network backbone consists of several Gigabit Ethernet links. Sunet's infrastructure is based on SRP rings. Internally, PDC uses Gigabit Ethernet over copper and fiber to connect the various clusters to PDC's core router pair. Other computers connected to the Net are storage servers, such as AFS file servers, HSM file servers, and of course, the backup server connected to the tape storage.

Unique for a high-performance computing center, when permitted by the batch system, PDC's users can make IP connections from and to all nodes on all clusters without the interference of firewalls or NAT. Neither does the network look any different on batch or login nodes. This makes life easier for PDC's users and administrators. The users experience a homogenous system that makes the step from test to production easier. The administrator does not need to bother with special hardware or configurations. This view of how the Net should be built results in a public IP address for every network interface on every node in every cluster, summing up to seven networks of size /24 advertised to the world. A /24 sized network has room for $2^{32-24} = 256$ IP addresses. Today PDC uses 11 subnets.

In reality, PDC has not used all 1792 possible addresses in its address space. Some of them are lost when the network address space needs to be divided into smaller subnets. Many usable addresses are lost when supercomputers are built with a number of nodes that are not a multiple of the power of two. To route IP packets between our subnets we use two main routers and some helpers, called cluster border routers. If there is an internal network in the cluster (and mostly there are such fast networks), these cluster border routers carry the traffic between, for example, the Myrinet inside Lucidor and the Gigabit Ethernet used on the outside.

But what is such a cluster border router? Even if specialized hardware exists, most cluster border routers are ordinary cluster nodes with additional software to perform additional tasks. As routing can decrease batch performance, login and other administratively used nodes are often "victims" to become cluster border routers. If wanted for redundancy, there can be several cluster border routers in each cluster. The routing protocol used internally between these routers is OSPF. It has several benefits: fast convergence, ease of set up, and several available implementations. The often-mentioned drawback of high CPU and memory usage is a myth still around since the time when routers had M68030 CPUs and 4 MB of memory. On hardware of the 21st century, as used in PDC's computing nodes, this is a true non-issue.

Further reading:
BGP:http://www.zvon.org/tmRFC/RFC1771/Output/index.html
GEANT:http://www.dante.net/server/show/nav.007
Giga Sunet:http://proj.sunet.se/gs/GigaSunet-rapport.pdf
KTHLAN:http://www.lan.kth.se
OSPF:http://www.zvon.org/tmRFC/RFC2328/Output/index.html
SRP:http://www.zvon.org/tmRFC/RFC2892/Output/index.html

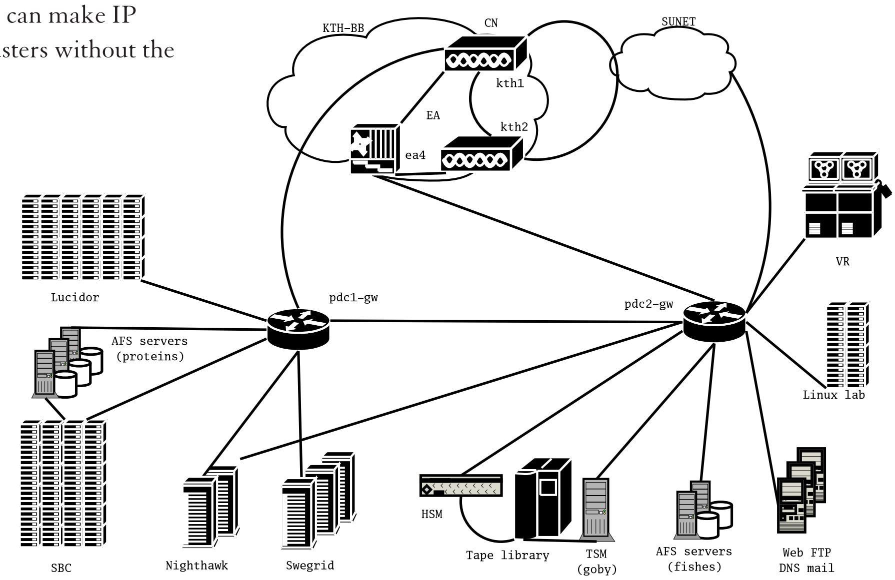


Figure: PDC network overview with connection to Sunet

Visualization of Unsteady Three-dimensional CFD Data

Stefan Görtz, Elias Sundström, and Kai-Mikael Jää-Aro, Department of Aeronautical and Vehicle Engineering, Royal Institute of Technology (KTH)

Large-scale simulations of three-dimensional, time-dependent flow fields are now commonplace in state-of-the-art Computational Fluid Dynamics (CFD). Such numerical simulations produce large amounts of flow-field data, often with several thousand discrete time steps. Each time step may require tens or hundreds of megabytes of disk storage, and the entire data set may be hundreds of gigabytes. Fluid flow features such as boundary layers, separation, recirculation bubbles, shocks, multiple vortices, and vortex breakdown are items of interest that can be found in the computed results. However, analyzing, visualizing, and communicating these unsteady 3D CFD results in 2D visualization environments is inherently difficult because of perceptual problems such as occlusion, visual complexity, lack of directional cues, and lack of depth cues. This has resulted in a rapidly growing need for 3D visualization tools. The computer system requirements for such tools are substantial. They include speed of computation, ability to quickly render high-resolution graphics, and massive data storage and retrieval capabilities.

The Virtual-Reality (VR) Cube at PDC is such a tool. It offers a fully immersive visualization environment, which displays synchronized images on all six surrounding surfaces of a room-sized cube. Several people wearing lightweight stereo glasses can enter and walk freely inside the VR Cube and see 3D images together. The main advantage over ordinary graphics systems is that the viewers are surrounded by the projected images, which means that the images are the users' main field of vision. This surround view adds to the immersion, as the peripheral vision is an important part of human orientation capabilities. A head tracking system continuously adjusts the stereo images in real time according to changes in the user's position and viewing angle. That is, perceptually, the user sees the virtual scene in a manner consistent with if it were real. The viewers can also see their own hands and feet as part of the virtual world. This gives them a heightened sense of being inside that virtual world.

The visualization software used in this project is VirCinity's COVISE software. COVISE, the COoperative VIsual Simulation Environment, is a modular and object-oriented software system for collaborative visualization sessions. Standard post-processing tools such as streamlines, pathlines, streaklines, iso-surfaces, and particle animation are available. These are computational analogues of the classical wind-tunnel techniques such as smoke injection, dye advection, time-exposure photographs, tufts, etc.

The VR environment has been evaluated by visualizing the flow field of different pre-computed solutions to the time-accurate Navier-Stokes equations, for example, the time-dependent flow over a full-span 70° delta wing at high angle of attack, the steady hypersonic flow around atmospheric reentry vehicles, and the steady airflow around a human female standing in a strong headwind.

The inherently unsteady flow over the delta wing was the original motivation to go into the VR Cube. For this reason, this case is presented here and we focus on demonstrating the benefits of visualizing this complex flow in the VR Cube.

Due to the high angle of attack, two burst vortices are present in the flow field over the delta wing. A standard technique for analyzing a vortical flow field is to look at the spatial and temporal development of vortex cores. Vortex cores are at the center of swirling flow. Vortex cores reveal vortex burst, which is characterized by a sharp kink in the vortex core filament. By releasing pathlines, streaklines, and animated particles into the computed flow field, the viewer can explore physical phenomena such as oscillations in the vortex breakdown location, or asymmetric vortex breakdown. For this purpose, a COVISE network with looping properties was created in order to load and animate 60 of the more than 1,500 time steps that were saved to disk. The network was configured to allow for setting interactive cutting planes, placing iso-surfaces and initiating particle traces from inside the VR Cube. Data reduction modules were used to load as many time steps as possible into the main memory.

Figure 1 shows an interactive visualization session inside the VR Cube. For this photograph, animation, head tracking,

Figure 1.

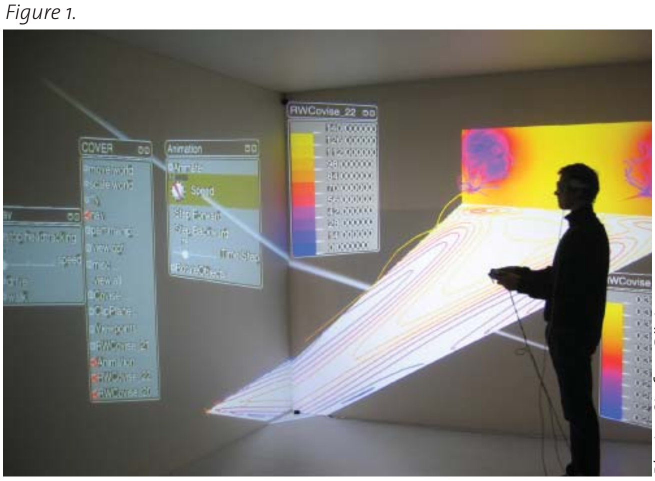


Photo: Stefan Görtz

PDC's Leading Roles in EGEE

The Enabling Grids for E-Science in Europe (EGEE) project started in April 2004 with PDC at KTH and the Swedish Research Council (VR) as the Swedish partners. Per Öster at PDC is appointed Regional Operation Center Manager for the Northern European Region. PDC will also propose, implement, and monitor the project's security architecture with Åke Edlund as appointed EGEE Security Head and Olle Mulmo as EGEE Chief Security Architect. More information can be found in the next issue of PDC Newsletter and at http://www.eu-egee.org and stereo viewing were switched off, making the display appear non-immersive. The COVER menu and the animation submenu are shown on the left wall. The delta wing and an instant in time of the corresponding unsteady flow field are projected mainly on the rear wall, together with color bars for the pressure coefficient and velocity magnitude. The flow field is visualized using a cutting plane colored by pressure coefficient, pathlines colored by velocity magnitude and pressure coefficient iso-lines on the wing's surface. Both the cutting plane and the pathlines are controlled interactively. Since the flow is pre-computed, it can be investigated at any length scale, and with control over time, for detailed analysis of long- and short-duration phenomena. In Figure 1 the user is seen changing the animation speed by intersecting a virtual "laser beam" extending from the 3D input device with the "speed" entry in the animation menu.

Compared to cheaper flat-screen visualization methods, the benefit of visualizing the flow field inside the VR Cube is that one can walk around the delta wing and explore the surrounding flow. When wearing stereo glasses, the delta wing seems to float in the middle of the room. The sheer sensual impact of the immersive display has a powerful effect on the physical intuition and makes it possible to gain a quick, intuitive understanding of the flow. Also, the collaborative environment of the VR Cube amplifies the human power for group problem solving and enhances communication.

In summary, we found that interactive tracing tools such as streamlines, moving points, pathlines, and streaklines are effective methods for depicting time-varying flow phenomena. Especially rapid vortex growth, which is difficult to visualize and communicate in 2D, is easily detected and displayed.

Another case that we visualized in the VR Cube is a steady-state Euler solution of the airflow around a human female standing in a strong headwind. Figure 2 shows a "rake" of streamlines and a color mapping of the surface-tangential flow velocity. This flow simulation was performed by Stephen Conway at the Swedish Defense Research Agency (FOI/FFA).

Clearly, one of the most important applications of the VR Cube is in communicating CFD solutions. Unsteady flow phenomena can be demonstrated and explained to people who do not have the interpretive skills needed to interpret flat-screen displays.

One disadvantage is that the VR Cube is a shared resource in a separate building. It has to be booked, and data must be transferred and set up. While this structure can support formal review, presentation, and detailed analysis of CFD solutions, it does not lend itself to casual or spontaneous visualization sessions.

The full version of this paper will be presented at the European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS 2004. Jyväskylä, Finland, 24–28 July 2004.

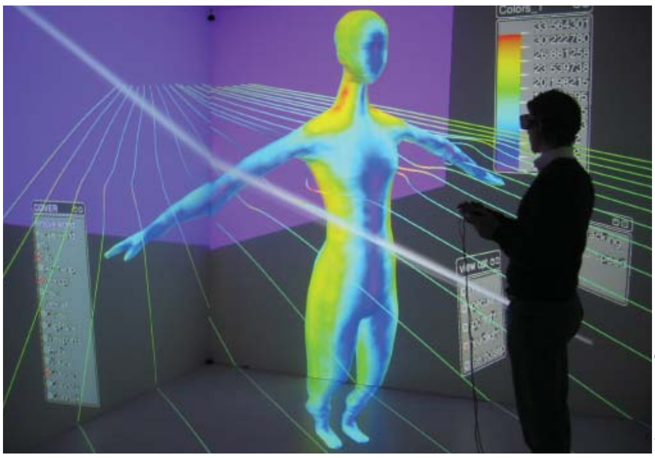


Figure 2.

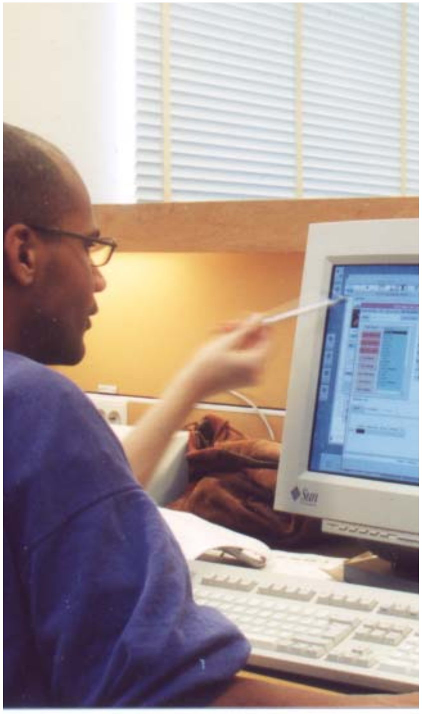
Photo: Stefan Görtz

Introduction to High-Performance Computing

The traditional PDC Summer School takes place August 16–27 at KTH.

This is an intensive two-week summer school course, for a limited number of participants.

A number of topics will be covered in overview lectures, in-depth technical lectures, and hands-on computer lab sessions.



A student working in a hands-on computer lab session at PDC summer school.

For more information, visit the Web site:

http://www.pdc.kth.se/training/summerschool

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PDC
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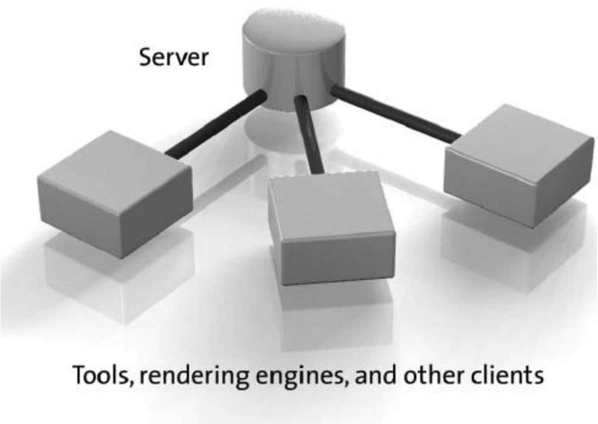
Uni-Verse: An Open Source VR Project

Gert Svensson, PDC

A three-year EU project, coordinated by PDC, was started in February. The goal of Uni-Verse, as the project is called, is to create an open source Internet platform for multi-user, interactive, distributed, high-quality 3D graphics and audio for home, public, and personal use. The platform will support high-quality 3D graphics as well as high-quality 3D audio and acoustic simulation. The platform will be scaleable from simple PDA's to large immersive environments. Its foundation is a unique lightweight, low-latency, general-purpose network protocol for 3D data, called Verse, developed by Eskil Steenberg and Emil Brink, then at the Interactive Institute, Stockholm, now at PDC.



A typical Verse architecture

The protocol lets multiple applications act together as one large system by sharing data over the network. If one application makes a change to the data, the modification is distributed instantly to all interested clients. Therefore, rendering engines, tools, simulation engines, and other components can be separate applications working together over a network to form a new application. This simple network protocol allows anyone to write components and applications that are compatible. The protocol is usually configured with a central server that acts as a hub passing messages to the clients. Clients no longer need to access data through load/save features. because all communication is done instantly using the protocol.

The components to be developed include advanced 3D graphics engines, tools, visual scripting, and a game engine. We will also integrate existing tools. A unique 3D audio acoustics simulator enables concurrent architectural and acoustical design in a distributed manner. The audio client will combine physical and perceptual modeling in a novel way to achieve a high performance level. The platform will be tested in two application areas, architecture and digital media, but the application of the platform is extremely wide and will have an impact on the interactive media industry as well as design, arts, education, and simulation.

The project funding is shared equally between the European Commission and the project partners, who are KTH, Sweden; the Interactive Institute, Sweden; Helsinki University of Technology, Finland; Fraunhofer Institute, Germany; Blender Foundation, the Netherlands; Paregos Mediadesign, a Swedish digital media company; and the architectural office MinusPlus from Hungary. The Blender Foundation in Amsterdam coordinates one of the largest open-source communities developing the Blender 3D tool.

Photo: Harald Barth

"The Verse technology makes a new way of thinking possible, with a more modular and collaborative design possible," says Blender Chairman Ton Roosendaal.