

PDC Newsletter

Visualizing the Year at PDC

The year of 1998 at Paralleldatorcentrum has been focused on visualization and virtual reality. Bids were sent out for construction of the VR-CUBE in the spring; the contract was signed in the summer; and the Cube was built and opened in the autumn. In November, PDC ran a collaborative application in the Cube in Stockholm and in the Argonne National Laboratory booth on the convention floor at SC98 in Orlando, Florida. To finish out the year, the theme for PDC's annual winter PDC conference was high-performance computing in visualization and virtual reality.

On October 23, 1998, King Carl XVI Gustaf of Sweden inaugurated PDC's VR-CUBE, a fully immersive six-surface CAVE-like system. Built by TAN Projektionstechnologie in Germany, the Cube is the first in the world to project images onto the floor and ceiling of a room, as well as the four walls. The system tracks a user's position and angle of sight, and the images that are projected onto the six surfaces change correspondingly.

The inauguration was an all-day event that began with invited talks from industrial scientists and artists about a variety of aspects and uses of virtual reality.

Later in the afternoon, about 350 people — including King Carl XVI Gustaf — listened to presentations from Björn Engquist, director of PDC; Janne Carlsson, president of KTH; and P. G. Hedström, chair of the PDC board of directors. Afterwards, the king visited the Cube: he walked through the Stockholm Exhibition of 1930, he experienced a scientific application of an airbag design from Daimler-Benz, and he viewed an art installation.

"There is a need for a coordinated research program in virtual reality in Sweden," said Engquist at the inauguration. "We are at the threshold of a revolution in this technology,



Johan Ihrén, PDC system administrator; King Carl XVI Gustaf; Peter Ullstad, architect in the KTH Architecture Department; and Janne Carlsson, former president of KTH, in the Cube during the inauguration.

and our goal at PDC is to create a center that integrates today's most advanced visualization systems into our supercomputing environment."

As many as ten people can participate in the Cube, whose floor is 3x3 m (approx. 10x10 ft.) and walls are 2.5 m high (approx. 8 ft.). It is powered by a Silicon Graphics Onyx2 with twelve R10000 processors and three graphics pipes.

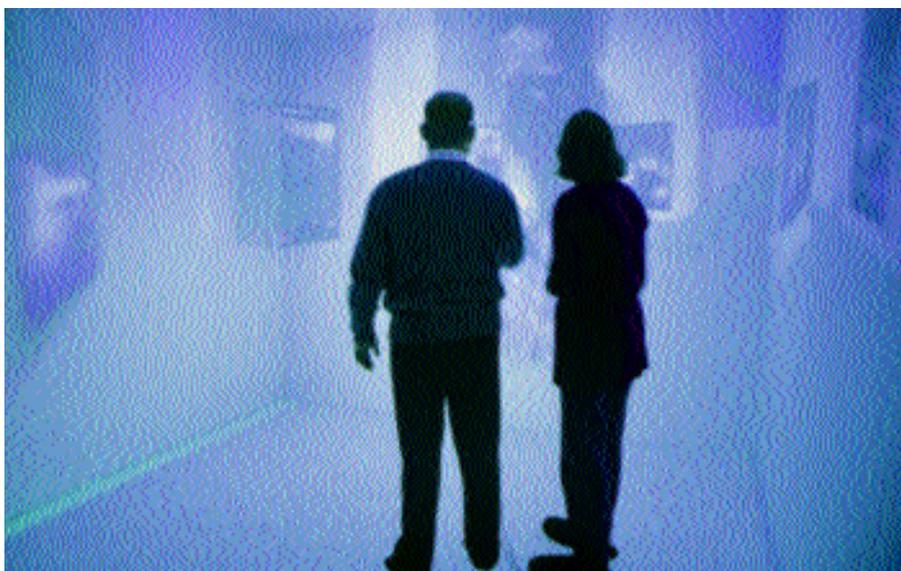
Uses for the Cube range from academic and industrial scientific research, to urban planning and architecture, to art. The PDC Cube is available to academic researchers and commercial enterprises throughout Sweden.

In This Issue

Visualizing the Year at PDC	1
From the Editor	3
PDC Progress Report 98	3
Visualization of CFD Computations	4
Building the Cube	8
PDC Annual Conference	10
README	10
HPCN TTN Network	11



Above: Four of the Cube's six surfaces can be seen here, as well as the navigation wand and 3D shutter glasses.



Left: Tom Coffin, of NCSA, and Margaret Watson, of Ars Electronica, in an art application in the Cube.

“Virtual reality gives industrial scientists the ability to work with complicated processes more easily,” said Hedström, who is also the corporate technical director of Electrolux. “This immersive visualization environment allows several people to simultaneously view scientific processes. Research findings can be viewed by a group, rather than only by one individual at a time, which facilitates more

meaningful discussions among researchers. This is a tool that can have an enormous impact both in academia and industry.”

The week before the inauguration included a two-day art workshop. Artists who use immersive visualization technologies met at PDC to share ideas, experiment with the Cube, and discuss the beginnings and direction of “virtual art.”

Guest artists included Margaret Watson, from Ars Electronica in Linz, Austria; and Tom Coffin, from NCSA in Urbana-Champaign, Illinois. The workshop was organized by Swedish artists Bino, Cybeard, and Cool.

Information and images about the Cube can be found on the Web at

<<http://www.pdc.kth.se/projects/vr-cube>>.

Contact <pdc-vr@pdc.kth.se> for further information.

From the Editor

King Carl XVI Gustaf of Sweden has now inaugurated the PDC VR-CUBE. It was built in record time, and all the relevant organizational, hardware, and software details worked extremely well on the opening day, October 23. Everybody who was involved in the project has the right to be proud. Interest from the public, the media, and of course the VR experts was overwhelming. We have decided to devote this issue of the PDC newsletter to virtual reality.

The VR-CUBE is the first six-surface immersive computational tool in the world, and it is a fantastic resource for 3D visualization. The combination at PDC of supercomputers and the Cube opens virtually infinite possibilities for applications in science and technology. Many phenomena are much better presented using high-resolution 3D techniques than using conventional graphics methods. A few examples are shapes of complex molecules, trajectories of particles, and three-dimensional flow fields.

The Cube joins the growing list of visualization tools available today. Many of its features make it uniquely useful in the areas of multimedia, visualization, and virtual reality.

All six surfaces of the room display computer-generated images, which completely surround the user. The room's size allows several users to experience an immersive environment simultaneously. Users can also introduce real-world objects into the virtual environment, to interact with virtual, computer-generated objects.

A vast number of academic disciplines can make use of the Cube. Researchers in everything from computational fluid dynamics, chemistry, and physics to psychology and sociology to economics and marketing can take advantage of the computational speed, storage, and visualization techniques available in the Cube.

Architects and urban planners can make enormous use of this technology, and industry holds great potential as well. Any type of machine or equipment design can be researched and developed in a 3D environment.

Today, art is an established and growing field in the world of visualization and virtual reality. The first event using the Cube was a

highly successful virtual reality art exhibition and workshop. PDC showed art applications in the Cube during the month of December, as part of the celebration of Stockholm as the European Cultural Capital for 1998.

One of the clear trends at the supercomputing conference SC98 in Orlando was the extensive use of 3D visualization. Applications of virtual reality techniques were common in many presentations. One of those applications could be seen in the Argonne National Laboratory booth. Johan Ihrén and Jonas Engström from PDC demonstrated a 3D flow visualization at the ANL booth in interactive sessions with researchers in the Cube in Stockholm.

I would like to extend an invitation to experience the VR-CUBE to all our readers. You are also very welcome to submit a proposal to PDC for a VR application in your own field of interest.

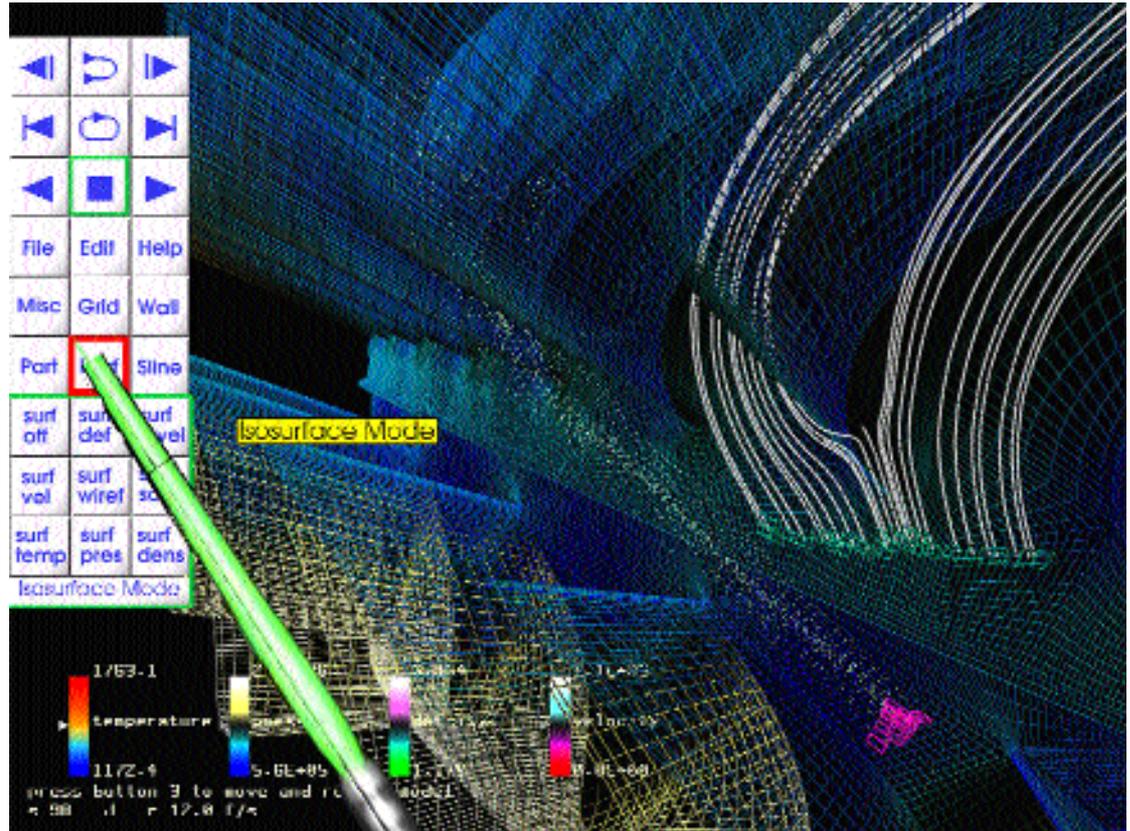
Björn Engquist
Director

PDC Progress Report 1998

Contributions for the *PDC Progress Report 1998* are now being accepted. As soon as possible, please send a title (even if it isn't the final one), the length of your contribution, the number of black-and-white images, and the number of color images, to pdcc-yearly@pdc.kth.se. We need the final text, all images, and complete bibliography information by January 20. The text should be in plain

text (ANSI/ASCII) format or LaTeX. Send formulas and tables either as printouts or as TEX-code to produce them. Black-and-white images should be in postscript, and color images should be in postscript or tiff format. Images should have captions, and captions for color images should have a more descriptive caption. All bibliography entries should include author, title, publisher, and year.

Fig. 1 The user interface for EnVis incorporates a pop-up menu that is made visible and hidden as desired. The 3D menu is fixed in the space of the Cube in any location the user feels is convenient, and it is easily moved when needed.



Visualization of CFD Computations

Jonas Engström, PDC

Overview

A software package called EnVis, or Engine Visualizer, has been designed and implemented as part of a CFD project carried out in cooperation between the Parallel and Scientific Computing Institute (PSCI), Volvo Aero Corporation (VAC), and Paralleldatorcentrum. The application is designed to visualize results from CFD computations.

Using immersive VR technology and parallel computations, it provides an interactive 3D visualization environment that can traverse large data sets quickly and easily, while maintaining a high level of interaction and immersion (see fig. 1). The application and its user

interface is designed to run in a CAVE-like environment. EnVis supports data sets produced by a Navier-Stokes solver called VOLSOL, developed by VAC.

Intended users are people with large VOLSOL-generated data sets and access to high-performance graphics computers. EnVis is designed to run on high-end ccNUMA-architecture computers (in this case, SGI) that are equipped with a projection-based VR system. The major application characteristics are:

- VOLSOL Data Sets** —EnVis uses VOLSOL grid files, command files, and solution files as input.
- CAVE Operation and User Interface** —all geometry-viewing, visualization, and user-interface operations are performed in a virtual environment (real or simulated) based on 3D projection.
- Solution Sequences** —fast animation of solution file sequences, along with associated visualization functions, is the primary feature of EnVis.
- Visualization** —support for basic visualization functions, such as vector arrows, streamlines, and traced particles, colored with scalar values like tem-

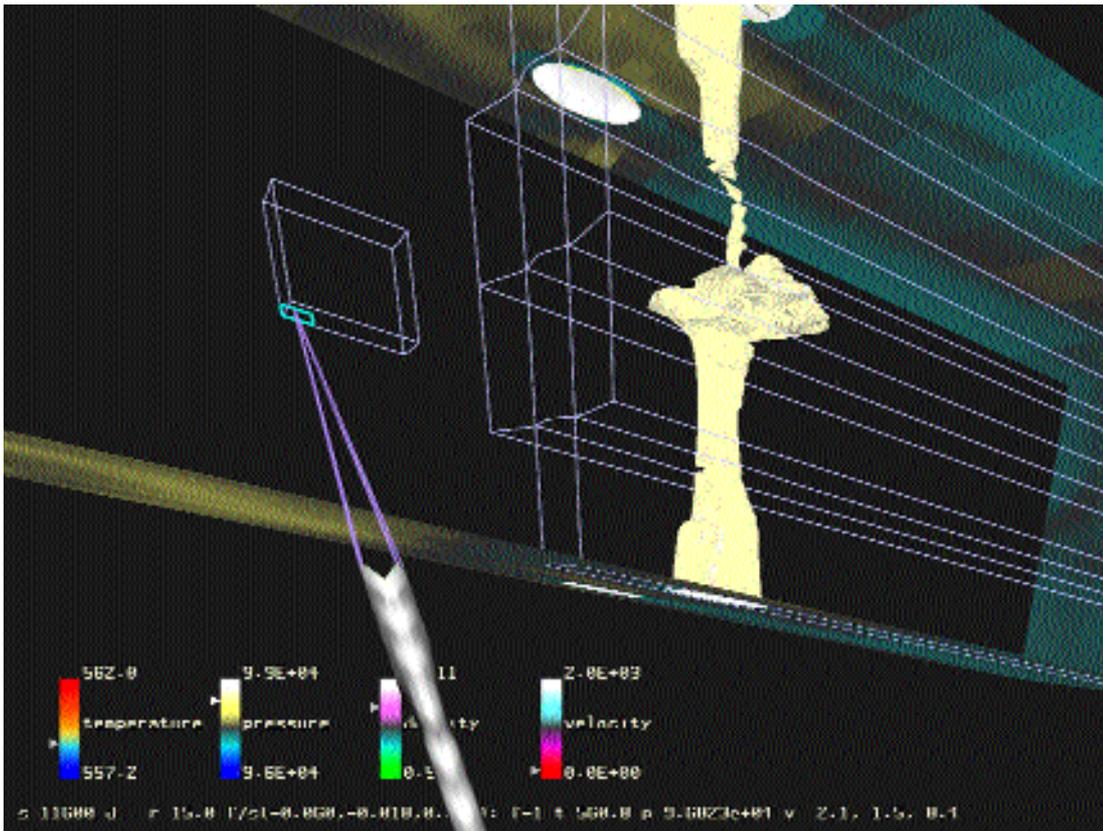


Fig. 2 Internal surfaces can be shown as outlines or as solid, as needed. They are shown here on an isosurface plot.

perature or pressure. In addition, isosurfaces can be rendered to show scalar values (see fig.2).

More information about EnVis is available in *EnVis User's Guide*, *EnVis Implementation Reference*, and the full version of this paper.

Processes and Data Flow

For performance reasons, EnVis uses multiple processes, a private solution file format, and multiple cache files for navigation and visualization functions.

The resulting data are then streamed through a number of EnVis processes that perform different tasks, such as importing data, updating particle positions, generating isosurfaces, and transferring final data to graphics hardware. The data path from VOLSOL to the end user can be described as follows (see fig. 3).

1. A user invokes EnVis once in file conversion mode, using VOLSOL output, to create preprocessed solution data suitable for fast importing. At the same time, cache files are generated for spatial search trees, geometry wall colors, and vector arrow

fields. These files are then used by all subsequent invocations of the program.

2. When all data files are in place, EnVis creates the following processes.
 - An importer process, which loads all the necessary data.
 - A number of rendering processes, which perform all the visualization computations not done by graphics hardware.
 - A number of display processes to handle user interaction and to transfer graphics primitives to hardware. The number of processes is equal to the number of walls in the CAVE.

In addition, The CAVE software, *CAVELib*, creates a number of additional processes for hardware interaction, etc.

Data Organization

The standard problem of navigating from Cartesian (x,y,z) to grid coordinates describing the indices of a particular cell has been addressed using a common approach for 3D spatial search problems; an oct-tree is used to perform binary searching in three dimensions. The leaves of the tree contain relatively

short lists of intersecting or enclosed cells that have to be searched.

In order to keep the redraw loop free from time-consuming operations — such as computations of streamlines, particle positions, isosurfaces, etc. — as much time-consuming work as possible is done by other rendering processes, and the redraw loop is “served” buffers containing points, line segments, and polygons.

An example of this is the implementation of wall coloring in which the walls in the geometry are colored using adjacent temperature or pressure. In this situation, the coloring of the walls changes with every time step, but the positions of the colored polygons remain fixed. The last wall property is used in combination with texture-mapping hardware to perform wall coloring (using a one-to-one mapping between polygon colors and pixels in texture memory). By computing all polygon colors in advance and storing them in a memory-mapped cache file, the update procedure is reduced to a single API call to copy data into a region of texture memory.

Fig. 3 Graphical representation of data as they are streamed through a number of EnVis processes that perform different tasks.

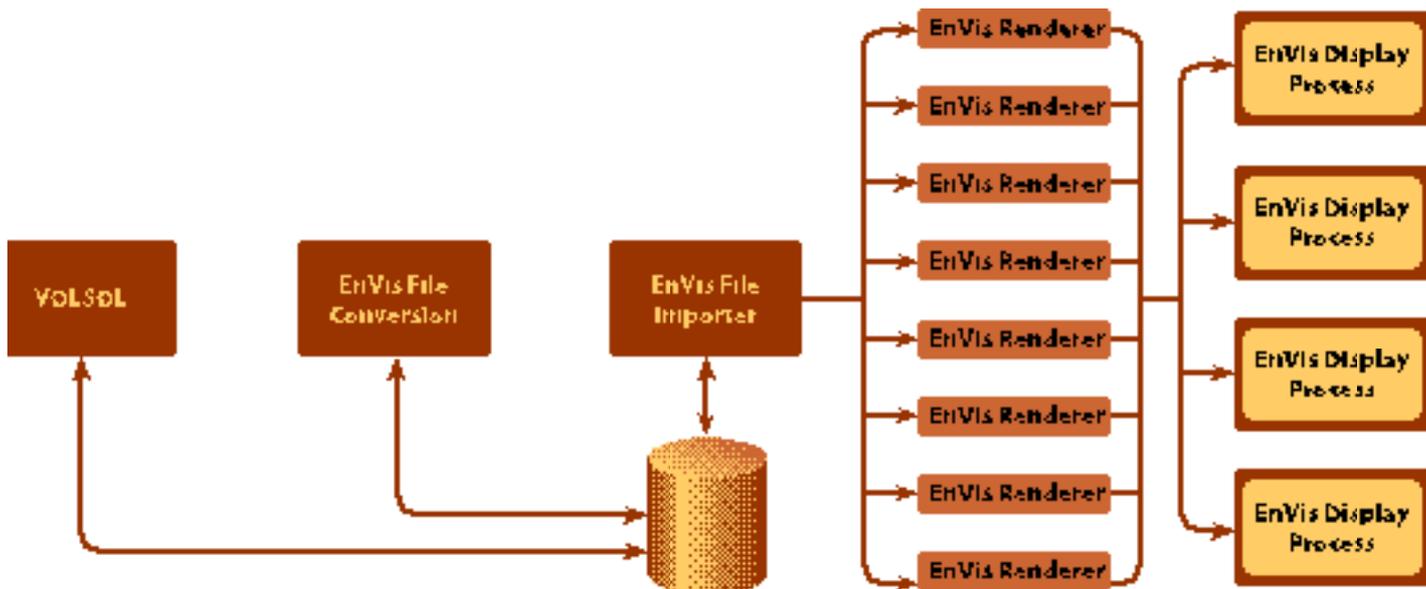
Visualization Performance

The major results of this project can be divided into 3D user interface development experiences and achieved visualization performance.

Most visualization operations performed by EnVis are dependent only on the information stored at the current time increment, which allows time steps to be rendered in parallel.

Data are organized in time-step-dependent and time-step-independent buffers. Time-step-independent data are tightly associated with visualization worker processes, where one process is tied to one buffer containing everything needed to build all graphics primitives for a time step. By using this scheme, visualization performance scales with the number of processors and available memory in the system.

In order to maximize overall performance, time-step-independent data are rendered at the coarsest possible level using one process per time step. This makes efficient use of multiple CPUs and available memory bandwidth, but at the cost of larger memory requirements.



The other category of visualization functions use information from sequences of time steps to illustrate flow, typically by combining data from the previous time step with the current one. This means that only a single time step can be rendered at a time due to data dependencies. Thus, parallelization must be implemented at a more fine-grained level. In order to achieve a high degree of parallelism — provided that work can be distributed to a number of potentially idling processes — a job queue for partitioned render work has been implemented. The rendering process puts all units of work in the queue, and all idling processes assist the renderer by processing work in the queue.

Table 1 shows an example of total speedups achieved when traversing a data set (1000 time steps, 8 GB total) with high numbers of activated visualization functions.

TABLE 1. Examples of speedup for different data dependencies

<i>Nproc</i>	2	3	4	5	6	7
Time step independent	1.5	2.0	2.5	2.9	3.4	3.8
Time step dependent	1.3	1.7	2.2	2.7	3.2	3.7

Future Work

Future work consists mostly of usability and performance enhancements. The single most requested feature is support for a common data file format, such as the widely used PLOT3D format. The second most wanted enhancement is a 2D GUI version of EnVis that runs on more affordable computer systems, such as high-end desktop workstations.

Support for showing multiple models simultaneously in the Cube has been considered, with local parameter scopes (using small visualization tools) to enhance application usability. The current visualization functionality can be extended with “surface-attached streamlines,” “contour surfaces,” and “clipping planes.” A natural extension to the current particle tracing functions is “trajectory lines,” showing the path of emitted particles. Level-

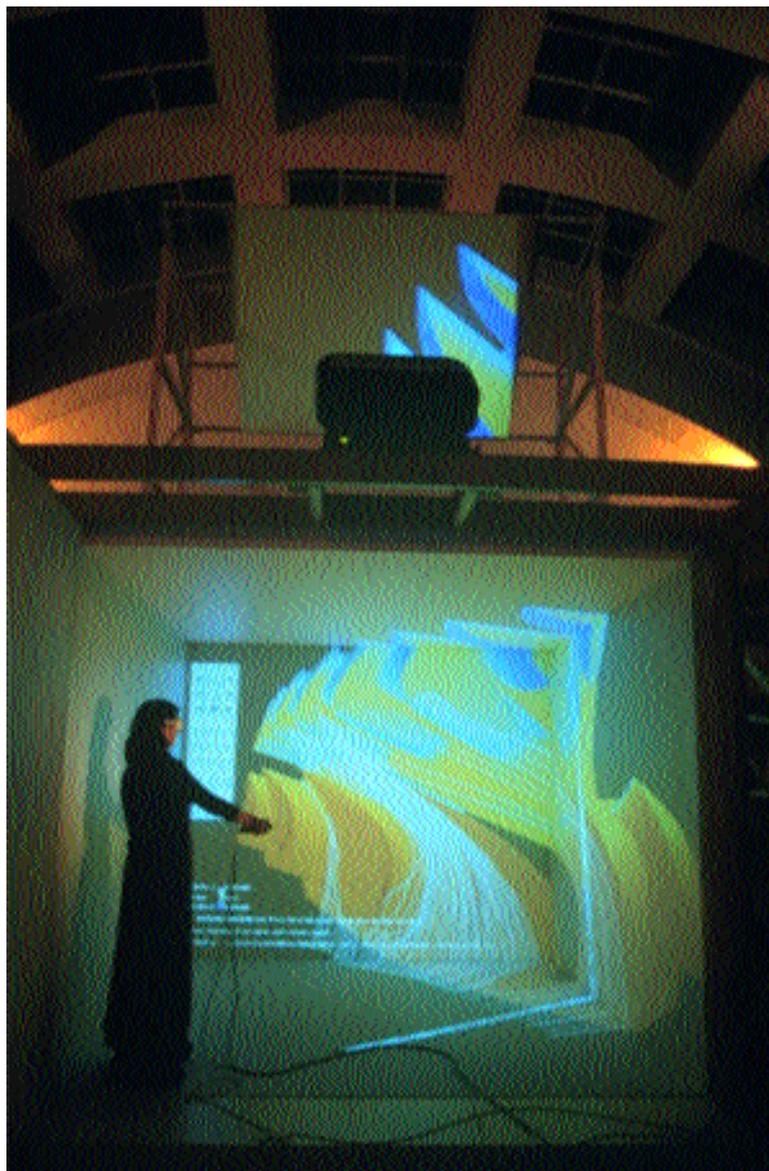


Fig. 4 User in the EnVis application in the Cube.

of-detail (LOD) performance optimizations have the potential to increase rendering speed dramatically and have already been partially implemented.

EnVis supports multi-user collaborative operation, where Globus software is used to address issues of security and reliable communication. We successfully demonstrated the collaborative capabilities of EnVis at SC98 in Orlando, Florida, in November of this year. Users in the Cube at PDC and on an ImmersaDesk in the Argonne National Laboratory booth on the SC98 convention floor navigated the application simultaneously. We hope to use this experiment as a starting point and continue to expand on this type of collaborative effort in the future.



The room where the Cube is located, before construction began.



Above: Members of the TAN construction crew attach the door to the frame of the Cube. Because the door is one of the image surfaces and must also open and close, it is hinged on the outside using wooden hinges.

Building the Cube

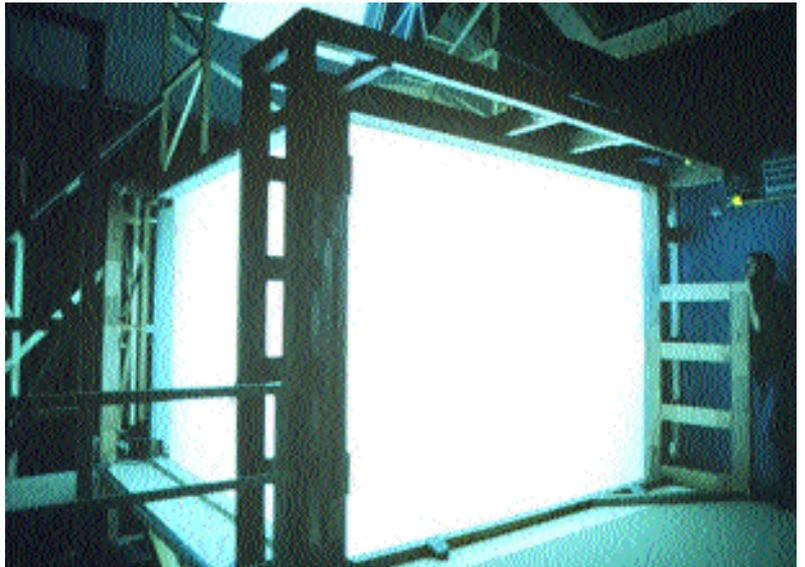
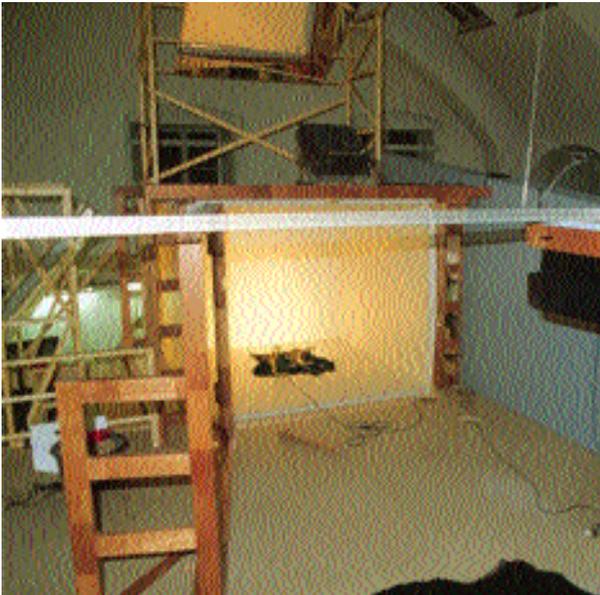


Above and right: The floor of the Cube is 250 cm above the floor of the building, to allow room for the equipment needed to project images onto the floor. Mirrors are used in projection. There are two mirrors for the floor, one for the ceiling, and one each for the walls not including the door. The longest beam of the substructure is 750 cm. Very little metal was used in construction, because magnetic metal might affect the tracking system. The beams are notched, and gravity and wooden nails are used to keep the structure in place.

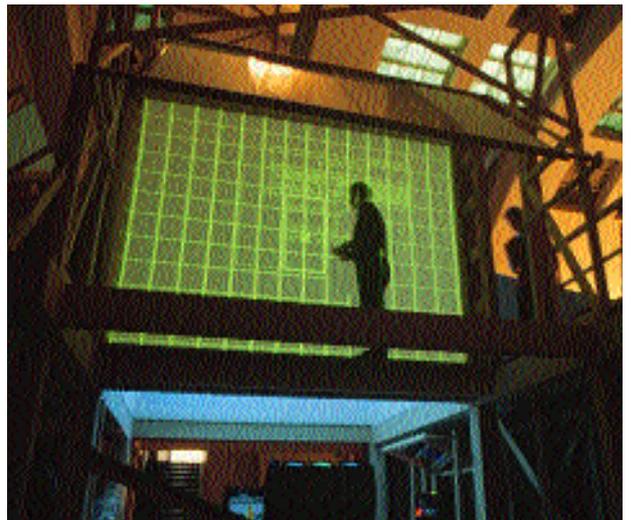


Above right: Transporting half of an SGI Onyx2, which is used to project the images onto the surfaces of the Cube, to the building.





Above left, and below left: The "walls" of the Cube are, in fact, projection screen material, which is stretched over the wall frames and tightened by attaching it to acrylic wedges and wooden pegs on the back side of the wall frame. The floor is made of 4-cm-thick acrylic, which is covered with this same projection screen material.



Above: A TAN engineer adjusts the projectors, by comparing a fixed straight line with a test grid projected onto the walls.

Left: Johan Ihrén, King Carl XVI Gustaf, Peter Ullstad, and Janne Carlsson, during the inauguration, navigating through a virtual 1930 Stockholm Exhibition – based on a 3D model created by KTH architecture students and transformed into a real-time application by Jörgen Netterlund at VRlab.



PDC Annual Conference

The 1998 Annual Conference carried on with the year's theme of visualization. *High-Performance Computing in Visualization and VR* was held December 17-18, on the KTH campus.

Among the speakers were

- Rachael Brady: National Center for Supercomputing Applications
- Thomas A. DeFanti and David E. Pape: Electronic Visualization Laboratory
- Thomas M. Jackman: IBM
- Peter Jacobson: VRlab, Umeå
- Gregory S. Johnson: San Diego Supercomputing Center

- Ulrich Lang: University of Stuttgart
- Thomas Reuding: BMW

Some of the topics of talks included *Global Tele-Immersion*, *Emerging Trends in HPC Visualization*, *Experience and Empathy in Virtual Reality*, and *Collaborative Scientific Visualization*.

More information about the conference can be found at <http://www.pdc.kth.se/news/events/conference98/> on the World Wide Web.

ä **Gaussian-98 is installed.** Gaussian 98 is installed on the IBM SP Strindberg and the Fujitsu VX/3 Selma. IBM SP users should note that there are now new key words for controlling parallel execution using Linda. For more detailed information, see <http://www.pdc.kth.se/compresc/software/>.

ä **SMP-parallel ESSL libraries.** The IBM ESSL libraries are now also available on the shared memory parallel (SMP) nodes on Strindberg. The library comes in two flavours: **esslsmp** and **essl_r**. Both are thread safe, but **esslsmp** has support for creating threads to allow for an otherwise single-threaded application to run the numerical library in parallel.

A typical compilation using **esslsmp** may look like `xlf90_r -q smp -lnoauto -lesslsmp`

For more information, see the IBM SP documentation at <http://www.pdc.kth.se/doc/>

ä **Updated versions of PESSL.** Updated versions of the MPI-parallel numerical library PESSL are available for testing. The new release includes a larger set of ScaLAPACK-compliant routines and are also using a calling convention compatible with more recent versions of ScaLAPACK. For more information, see <http://www.pdc.kth.se/doc/SP/manuals/peSSL> and contact pdc-staff for information on how to access it.

ä **CapTools.** Within the framework of an EC project, PDC is able to offer its users access to the parallelization software CapTools and its communication library CapLib. Usage is limited to PDC computers. More information about the programs is available at <http://captopools.gre.ac.uk/>. Interested users are encouraged to contact pdc-staff@pdc.kth.se.

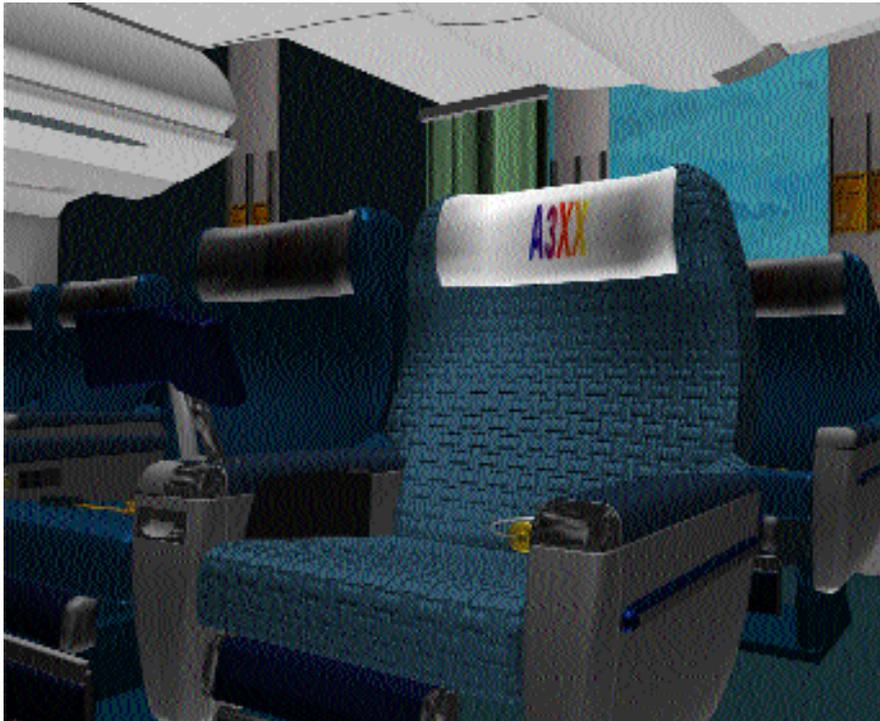
ä **EASY job statistics.** The EASY scheduling system is continuously developing at PDC. We are now able to offer post-analysis performance reports. These analysis reports are based on the state of the IBM SP node before and after your job. For more information, type the command **spjobstatistic** and see our Web information at <http://www.pdc.kth.se/support/easy-tour.html>.

ä **ABAQUS/5.8.** The new version of the solid mechanics software ABAQUS has been installed. This version is available on the computers Kallsup and Strindberg. The release includes the new post-processing program ABAQUS/Viewer, which will eventually replace ABAQUS/Post.

ä **CHARMM.** CHARMM is a program for macromolecular energy minimization and dynamics calculations. The program is available for PDC users after they register with the Department of Chemistry at Harvard. PDC has recently updated to version c25b2. For more information, see <http://www.pdc.kth.se/compresc/software/> and <http://www.pdc.kth.se/doc/charmm/c25b2/>.

ä **MacroModel/BatchMin.** The molecular dynamics package MacroModel/BatchMin is being updated to version 6.5. This process should be completed by the time of the distribution of this issue of PDC Newsletter. More information is available at <http://www.pdc.kth.se/compresc/software/> and <http://www.pdc.kth.se/doc/>.

ä **On-line course materials.** The PDC Web pages contain quite a bit of material from classes and tutorials being held at PDC. Soon, we will also introduce interactive courses in different aspects of HPCN. Stay tuned to <http://www.pdc.kth.se/training/> for more.



Reports on user requirements and on the current state of VR are available free on charge on the World Wide Web at

<www.syseca.thomson-csf.com/simulation>

The prototypes can also be demonstrated in Paris at SYSECA upon request to

<pierre.bouchon@syseca.thomson-csf.com>.

VR for Europe

VR for Europe is a project to promote the use of virtual reality technology in European industry. The project is performed by SYSECA, S.A., and is funded by the European Commission, Directorate General III Industry.



Prototypes of VR applications have been built from actual user specifications and requirements. These prototypes are being demonstrated at Technology Transfer Nodes across Europe, including a CAVE-like environment at a Dutch TTN in Amsterdam, and the VR-CUBE at PDC.

The general idea behind the prototypes is to show state-of-the-art VR and at the same time convey the idea that this field is evolving extremely rapidly. We hope that each prototype will be thought provoking and challenging to both the user and the developer by raising interesting and controversial issues about VR.

With these prototypes several aims are pursued at the same time. We present the current state of the art in VR, for those new to the field. We show that this is not a field with completely established solutions. We challenge conventional VR thinking for more VR-knowledgeable users.

The prototype being shown in PDC's Cube is an interactive 3D rendition of an aircraft interior. The interior is to be shown to prospective clients of Airbus Airlines. The goal is to show a wider variety of interiors than would be possible with a physical mockup, with the capability to test alternative designs for the interior.

Users are immersed in the aircraft interior, and they can change various ambiance parameters (night/day), fabric textures, and climate (warm/cold). Although the environment is immersive, it can also be viewed on a screen monitor if that is the only visualization equipment available.

B

Sverige
Porto
Betalt

PDC Newsletter

Published quarterly by Paralleldatorcentrum 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 Planning and Coordination of Research (FRN), and KTH.

Editor: Björn Engquist

Editorial staff: Faith Short

E-mail: pdcc-quarterly@pdc.kth.se

ISSN 1401-9671

How to Contact PDC

Visiting address: Lindstedtsvägen 3, Plan 5, KTH, Stockholm

Mail: PDC,KTH;SE-100 44 Stockholm;SWEDEN

E-mail: pdcc-staff@pdc.kth.se

WWW: <http://www.pdc.kth.se/>

Phone: +46 8 790 79 07

Fax: +46 8 24 77 84

PDCTTN

Contact: Marina Backer Skaar

E-mail: pdcttn@pdc.kth.se

WWW: <http://www.pdc.kth.se/pdcttn>

Phone: +46 8 790 69 23