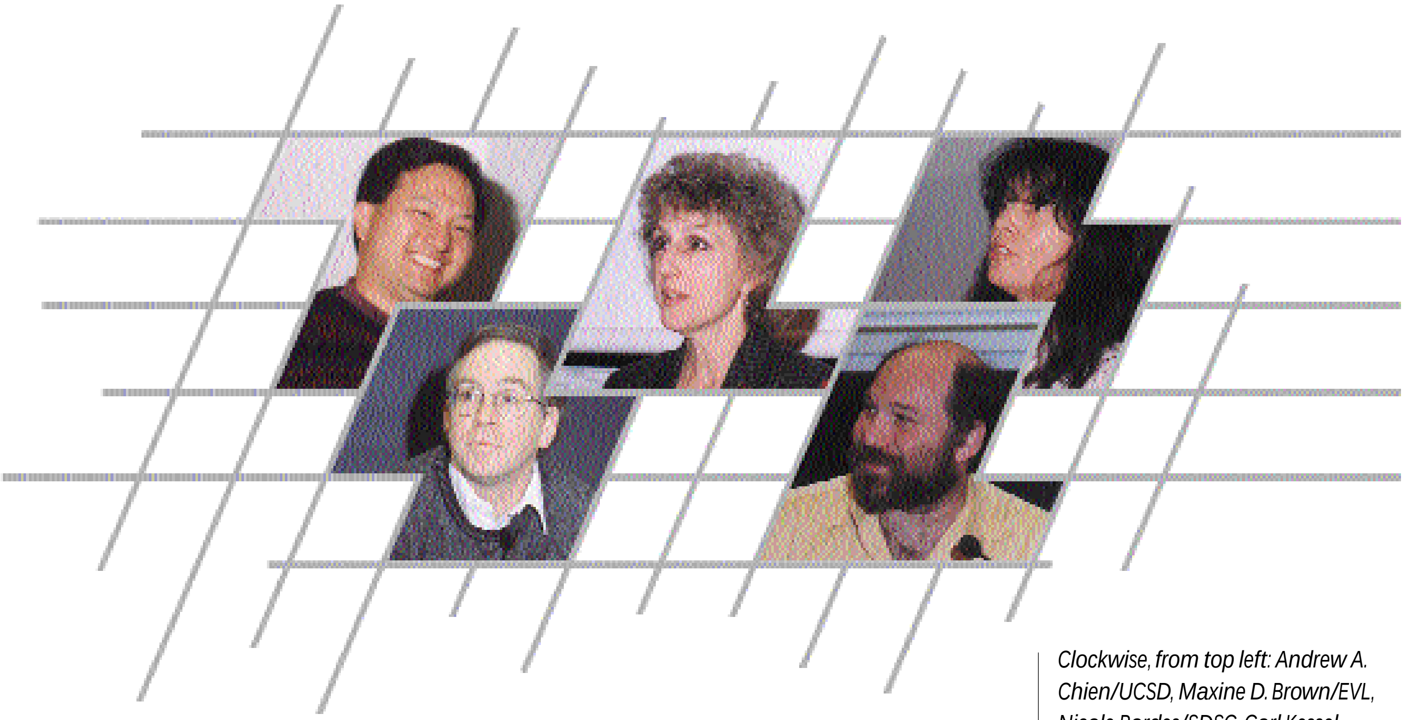
PDC Newsletter

Exploring the Grid



Clockwise, from top left: Andrew A. Chien/UCSD, Maxine D. Brown/EVL, Nicole Bordes/SDSC, Carl Kesselman/USC, Tom DeFanti/EVL

The seventh annual PDC conference, *Simulation and Visualization on the Grid*, from December 15–17, was distinctive in many ways. The conference included an additional day, with previous conferences lasting two days. This year, presentations of technical papers were included in the three-day program, along with presentations by invited speakers.

The biggest difference was the publication, for the first time, of the conference proceedings. As volume 13 in the Springer-Verlag series, *Lecture Notes in Computer Science and Engineering*, these proceedings contain the presentations and a transcript of the lively panel discussion from the conference. “We are very pleased to be in this series, and we’re looking forward to a continuing relationship with Springer,” said PDC director Björn Engquist.

The eleven invited papers included such topics as high-performance algorithms, working in cyberspace, supercomputing with clusters, and the Grid’s role in virtual reality. The researchers for the fifteen technical papers came from Europe, Asia, and North America; and their subject areas included astronomy, chemistry, computer graphics, physics, and virology.

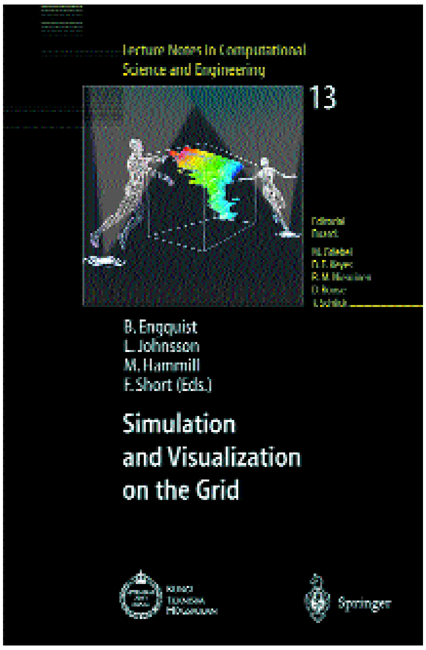
The presentations covered such Grid technologies as distributed file I/O, clustering,

Invited Speakers

Nicole Bordes — SDSC
Maxine D. Brown — EVL
Tom DeFanti — EVL
Andrew A. Chien — UCSD
Henry Fuchs — UNC
Fred G. Gustavson — IBM
Carl Kesselman — USC/ISI
Bernard A. Pailthorpe — SDSC
Thierry Priol — IRISA/INRIA
Dave Turek — IBM

In This Issue

Exploring the Grid 1
Board Members 2
New Nighthawk Nodes 3
README 3
Bioinformatics Infects PDC 4
Calendar of Events 6
HPCN TTN Network 7



Lecture Notes in Computational Science and Engineering

13

B. Engquist
L. Johnsson
M. Hammill
F. Short (Eds.)

Simulation and Visualization on the Grid

Springer

CORBA, software infrastructure, tele-immersion, interaction environments, visualization steering, and virtual reality.

Applications in biology, chemistry, and physics will benefit from the Grid; and the techniques used in such applications will help realize the power of the Grid.

On the final day of the conference, five of the speakers participated in a moderated panel discussion, "The Grid: What's Really Going On?" The panel members, experts in networking and applications on the Grid, addressed current successes and pitfalls of the high-performance computational Grid, as well as issues of the next millennium.

The 2000 conference, December 14-15, will be *Simulation and Visualization in the Life Sciences*.

More information about the PDC Conference Series is available on the Web at <**http://www.pdc.kth.se/conference/**>.

Authors of Technical Papers

Christer Andersson — KTH, Sweden
R. Holland Cheng — KI, Sweden
Bertil Dorch — SU, Sweden
Erik Elmroth — UU, Sweden
Erik Engquist — KTH, Sweden
Christer Fureby — FOA, Sweden
Bogdan Hnat — U.of Warwick, England
Malek O. Khan — LU, Sweden
Sungye Kim — Chung-Ang U., South Korea
Anton H.J. Koning — SARA, The Netherlands
Ottmar Krämer-Fuhrmann — GMD, Germany
Martin Kücken — U.of Potsdam, Germany
Per Linse — LU, Sweden
André Merzky — ZIB, Germany
Michael E. Papka — ANL,USA

Board Members

At long last, in the middle of their very busy three-year terms, PDC's board members were all in the same place at the same time for a photograph. PDC wants to thank them for their continuing outstanding service — and especially for their willingness to watch many flashbulbs explode early in the morning.

The three new members and four returning members represent academia, government, and industry. Their backgrounds include mathematics, chemistry, biology, and engineering. This wide range of experience brings an important variety of comprehension and balance to their decisions about scientific computing in Sweden.

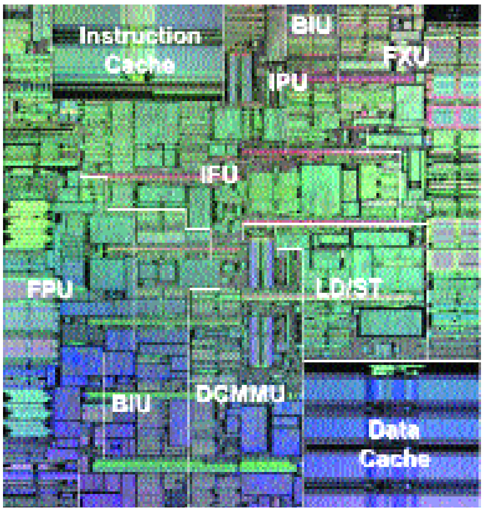
Standing, left to right: *Hans Wallberg, Anders Eriksson, P. G. Hedström, Gustaf Söderlind*

Seated, left to right: *Anne-Marie Pilotti, Gunnar von Heijne, Kersti Hermansson*

New Nighthawk Nodes

The new Nighthawk nodes in the IBM SP, Strindberg, have the following important features.

- 8 CPUs per node share the same memory
- 4 GB of memory per node (one node has 16GB of memory)
- 16 GB of **/scratch** file space for intermediate files
- Newer version of the IBM Fortran compiler
- New functionality in the object file archiver `ar`
- Shared GPFS parallel high-performance file system, which is shared between the new nodes but is not shared with the older nodes in the IBM SP
- Batch jobs must be submitted from <**strindberg.pdc.kth.se**> or <**august.pdc.kth.se**>. It is not possible to submit jobs from any of the interactive Nighthawk nodes.
- 2 new node types are available in the EASY commands. *N-nodes* are Nighthawk nodes with at least 4GB of memory. The Nighthawk node with extra memory installed is labeled *H*.
- With the current switch, up to 4 processes can share the switch interface in User Space mode. This means that inter-node MPI jobs are limited to a maximum of 4 MPI processes per node, if User Space is chosen as the communication library.
- To address more than 2GB of heap memory or more than 256MB of stack space in one program, the code must be compiled in 64-bit addressing mode.



Node comparison

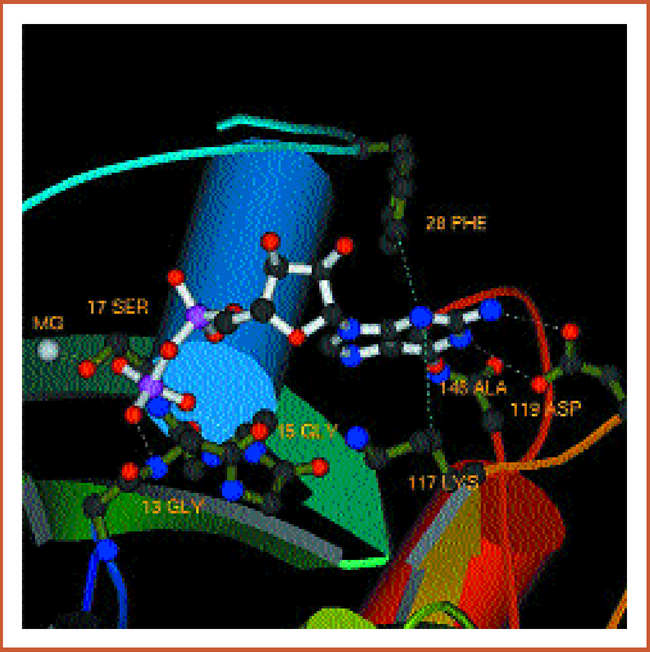
Type of node	*66 MHzWide*	*Nighthawk*
Installed at PDC	1994	2000
Form factor	Wide node	High node
Procs/node	1	8
Processor Architecture	POWER2	POWER3
Processpr MHz	66	222
Peak Mflop/s per proc.	266	888
Peak Gflop/s per node	0,266	7,104
Peak Aggr Mem BW GB/s	2,5	16

Complete information about Strindberg's system performance can be found through the PDC homepage, choosing "Computing Resources" and then "Hardware."

For more details, see <**http://www.pdc.kth.se/support/ Nighthawk-tour.html**>.

README

- **Practical MPI programming** And many other books related to computing in general and the IBM SP in particular can be found in the IBM red book collection <**http://www.redbooks.ibm.com/**>
- **Fortran90 transition** Thinking about converting your code to Fortran90 but stagger at the amount of work required? The tool FORESYS might be a valuable resource available to you as a PDC user. <**http://www.pdc.kth.se/compresc/software/**>
- **Hard-to-track F77 bugs?** The `-qextchk` flag of the IBM xlf compiler can help you track problems regarding incorrect parameters to subroutines and inconsistently declared common blocks. <**http://www.pdc.kth.se/doc/**> Also, FORESYS is a tool that detects similar errors.
- **Suggested reading** Looking for the perfect gift? You can find suggested reading material on high-performance computing at <**http://www.pdc.kth.se/training/references.html**>.



Bioinformatics Infects PDC

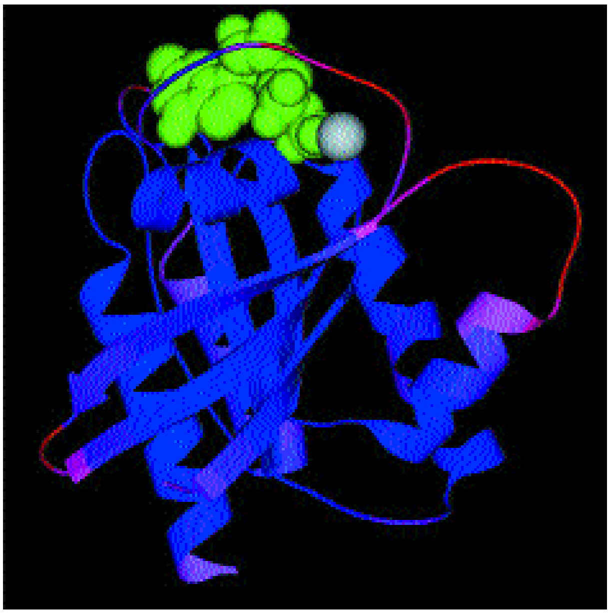
In the spring of 2000, the Knut and Alice Wallenberg Foundation awarded 7.5 million Swedish crowns (MSEK) for bioinformatics development to Gunnar von Heijne and Björn Engquist. The grant will be awarded over 5 years, at 1.5 MSEK per year, and is part of an 800 MSEK grant for functional genomics.

Professor of biochemistry at Stockholm University, von Heijne is the head of the Stockholm Bioinformatics Center (SBC) – a national facility designed to provide a critical mass of bioinformatics and computer science expertise for high-level research, methods development, and advanced post-graduate training in bioinformatics. Engquist, professor in the department of numerical analysis and computing science, is the director of Parallelldatorcentrum (PDC), Sweden's major high-performance computing center.

Together, SBC and PDC will build an initial cluster of personal computers; this will incrementally become a supercomputer, made up of 100–200 PCs, for bioinformatics. As they learn more about how to use these machines, they will continue adding to the cluster.

"The initial cluster will be built during the fall of 2000," according to von Heijne, "and our two groups are now planning the best way to integrate the current computing environments at Stockholm University and PDC."

Bioinformatics is the application of computer science and technology to problems in the biomolecular sciences. It is one of the key areas in the present data explosion in biology brought about by the genome projects and the new developments in functional genomics and proteomics.



Schematic image of the 3D structure of the protein ras p21, which is involved in growth signalling within cells. In a large fraction of human cancer cases, this molecule has been mutated and no longer responds properly to signals. Using bioinformatics methods, a large number of similar proteins have been identified, many of which are involved in different kinds of biological signalling processing.

Left: *View of the protein backbone with the bound GDP molecule and Mg ion.*
Middle: *Closeup view of the GDP binding site.*
Right: *The protein backbone is coloured according to flexibility (where blue is stiff, red is flexible).*

The solution structure of ras p21 was determined by Per Kraulis et al (*Biochemistry* 1994, vol 33, pages 3515-3531), and the image was generated using MolScript <**http://www.avatar.se/molscript**>

The Human Genome Project, an international project to identify all the genes of the human body, is one of the prime examples of this combination of technology and biology. The existence of the human genetic map will lay the foundation for a revolution in medical diagnosis and treatment.

Bioinformatics research and methods development are currently expanding rapidly in Sweden. Von Heijne describes the area as "the use of computer technology to handle, analyze, and add value to the flood of data coming out of modern genomics and proteomics research." The field includes such applications as information processing (storage, retrieval, and analysis) and modeling biological and behavioral processes.

Research at SBC is focused in three areas: protein sequence and structure, molecular evolution, and modeling of cellular function.

Researchers can analyze and make predictions about protein structure from the amino acid sequence. These kinds of predictions can aid in areas like drug design for pharmaceutical development. The analysis and comparison of whole-genome data is a very important aspect of such studies.

Molecular evolution looks at how proteins have evolved and how organisms are related to each other. Using the PC cluster, scientists have opportunities for data-mining protein family databases and DNA sequence databases, among others. There are masses of these kinds of data, and this type of research has many implications. "For example," says von Heijne, "we can begin to make evolutionary deductions about bacteria, which is important in the health field, given the increasing numbers of drug-resistant strains of bacteria."

Another use of the cluster, according to von Heijne, is to develop models of signaling networks in cells, which can shed light on how genes are turned on and off. "We can study metabolic responses at the cellular level, to gain a comprehensive view of the cell from a theoretical perspective."

For more information, see <**http://www.sbc.su.se**>

Calendar of Events

October

12–14 Applied Mathematics for Industrial Flows, 2d International Conference
Il Ciocco; Tuscany, Italy
http://dmawww.epfl.ch/Quarteroni-Chaire/AMIF/AMIF2000/

16–17 High-Performance Graphics Systems and Applications European Workshop
Bologna, Italy
http://www.cineca.it/events/HPGraphic/

17–19 Advanced CAVE Workshop Series
Old Dominion University; Norfolk, Virginia
http://calder.ncsa.uiuc.edu/CAVERNUS_Workshop/

19–20 Photophysics and Photochemistry 2000
Oeiras, Portugal
http://www.itqb.unl.pt/pp2000/

22–25 VRST'2000: ACM, SIGGRAPH, and SIGCHI Symposium on Virtual Reality, Software, and Technology 2000
Seoul, Korea
http://vrst2000.kist.re.kr/

23–25 CIMASI'2000:3d International Conference on Applied Mathematics and Engineering Sciences
Casablanca, Morocco
http://www.cimasi.org.ma/

November

6–9 PDCS 2000:12th IASTED International Conference on Distributed Computing and Systems
Las Vegas, Nevada
http://www.iasted.com/conferences/2000/lasvegas/pdcs.htm

6–10 SC'2000
Dallas, Texas
http://www.sc2000.org/

15–16 Workshop for Swedish Ph.D. Students and Postdocs in Bioinformatics
Uppsala University, Sweden
http://linnaeus.bmc.uu.se/workshop_reg.html

28–Dec 2 Cluster 2000: International Conference on Cluster Computing
Chemnitz, Germany
http://www.tu-chemnitz.de/informatik/RA/cluster2000/

December

14–15 Simulation and Visualization in the Life Sciences
KTH, Stockholm, Sweden
http://www.pdc.kth.se/conference/2000/

17–20 HiPC '00:7th International Conference on High Performance Computing
Bangalore, India
http://www.hipc.org/

17–20 GRID'2000:1st International Workshop on Grid Computing
Bangalore, India
http://www.gridcomputing.org/

January 2001

3–6 HICSS-34: Hawaii International Conference on System Sciences
Maui, Hawaii
http://www.hicss.hawaii.edu/

February 2001

6–8 Advanced CAVE Workshop Series
University of Puerto Rico
http://calder.ncsa.uiuc.edu/CAVERNUS_Workshop/

19–22 AI 2001:IASTED International Conference on Applied Informatics
Innsbruck, Austria
http://www.iasted.com/conferences/2001/austria/ai.htm

19–22 MIC 2001:IASTED International Conference on Modelling, Identification, and Control
Innsbruck, Austria
http://www.iasted.com/conferences/2001/austria/mic.htm

April 2001

11 Advanced CAVE Workshop Series Demonstration Seminar ACCESS
University of Puerto Rico
http://calder.ncsa.uiuc.edu/CAVERNUS_Workshop/

July 2001

9–13 8th IFIP TC13 Conference on Human-Computer Interaction
Tokyo, Japan
http://www.interact2001.com/

29–Aug 1 ICAD 2001:7th International Conference on Auditory Display
Helsinki University of Technology; Espoo, Finland
http://www.acoustics.hut.fi/icad2001/

October 2001

14–19 ICHMT Symposium on Visualisation and Imaging in Transport Phenomena
Antalya, Turkey
http://ichmt.me.metu.edu.tr/upcoming-meetings/Vim-01/announce.html

KneesUp Lowers Pain

Orthopedists require the greatest accuracy to develop prosthetic implants for human menisci, in order to avoid problems from wear during a long lifetime. Current total knee-joint replacements are designed to reduce pain in elderly patients' arthritic knees. These replacements do not function well at the level required by highly physically active patients, because premature wear leads to further joint damage. The cost benefits and improvements to patient care from the improved design of such prosthetics are clear.

KneesUp represents the first realistic 3D model of the human knee joint, including soft tissues, specifically designed to investigate the biomechanical environment of the menisci. This model can be used to design prostheses through the study of test cases that include normal walking, injury, and impact scenarios. KneesUp can also improve the effectiveness of virtual crash-test dummies, by studying the effects of automobile crashes on the knee joint.

The menisci of the knee are two horseshoe-shaped pieces of fibrocartilage that help transmit load evenly from the thigh bone to the shin. Damaged menisci do not repair naturally, and usually the only treatment option is to remove all or part of the meniscus. This produces well-recognized degenerative changes in the joint, leading to osteoarthritis. Many patients with meniscal injuries return with arthritic pain one or two decades later.

The KneesUp model is based on highly detailed geometric data from Magnetic Resonance Imaging (MRI) scans of cadaveric specimens. Algorithms were designed to identify the tissue type within the MRI scans. The project partners then generated a 3D model and remeshed the vital soft tissues to solid representations, using published research and laboratory experiments to link the material properties of the specimen with the model.

Further information can be found through "Success Stories" at <**http://www.hpcn-ttn.org**>.

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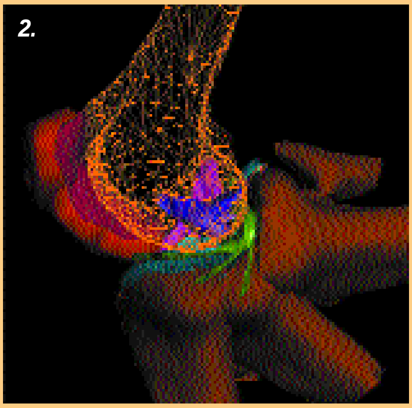
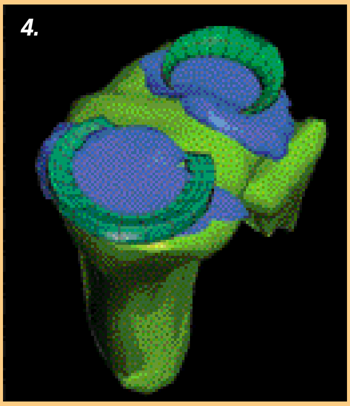




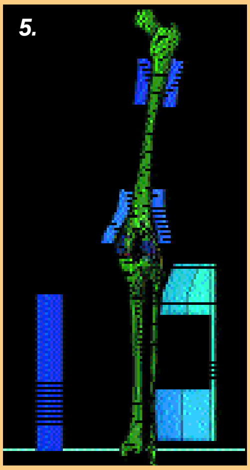
__1.__ PAM-SAFE simulation of a pedestrian frontal knee impact, showing the knee joint.

__2.__ PAM-SAFE walking simulation (gait cycle),using simplified hamstring and quadriceps tendons as cable elements.

__3.__ Accurate 3D Model of the human knee joint (anterior view).

__4.__ Meniscal implant study, approximation of both menisci shapes.

__5.__ PAM-SAFE simulation of a pedestrian frontal knee impact, showing the whole leg.



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PDC Newsletter

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