

PDC NEWSLETTER

New HPDR Contract

On May 14 KTH and HPDR signed a 77 MSEK contract for the funding of PDC during 1997-1999. This is the largest contract KTH ever entered for a single purpose. Of the known funding for HPDR about 2/3 will be invested in PDC during these years. "The decision clearly shows HPDR's trust in PDC" says PDC Director Björn Engquist. "This will help us attract new partners and additional funding from other sources."

Background

The Swedish Council for High Performance Computing (HPDR) was formed in 1994 to rectify that Sweden was lagging behind in high-performance computing.

After an international evaluation HPDR decided to invest in a build up of parallel computing capacity at PDC and also in continued vector investment for a limited period at NSC in Linköping. This led to a initial HPDR-KTH contract totaling in 43 MSEK requiring an extensive and rapid expansion in only 18 months of the staff, organization and infrastructure as well as computational resources. Much emphasis was given to operational aspects with high requirements on availability but also high requirements on user support. This led to a doubling of the staff and a dramatic expansion of the IBM system up to 110 faster nodes with more memory per node. The networking and storage infrastructure was also heavily expanded. In our opinion this has resulted in a super-computer center of international class.

The result from this rapid expansion was evaluated of another expert committee in the fall of 1996 with excellent



The Contract is signed by KTH President Janne Carlsson (middle), HPDR Chairman Sonja Dahl (left) and Director of HPDR Secretariat Anne-Marie Pilotti (right).

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result. PDC was found to have completely fulfilled every aspect of the original proposal. Based on this HPDR decided to invest most of its funding at PDC.

The contract makes it possible for PDC to offer its resources free of charge to the academic community while industry have to pay full price. Projects with funding from NUTEK or the EC are charged a reduced fee.

PDC Conference Call for papers

The theme for the traditional PDC December conference 18-19 December 1997 is "Novel Areas of High Performance Computing". Extended abstract following the theme should be submitted before October 13. There will also be a session for PDC users presenting projects.

See www.pdc.kth.se/news/events/events.html for more information.

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For the first time it is possible for PDC to plan for a somewhat longer time than the immediate future. As you see on the cover page, HPDR and PDC/KTH has now signed a contract for the period 97-99. PDC will play a leading role in the development of high performance computing with academic applications during the next few years.

As part of the planning process the board of PDC invited HPDR to a meeting on June 16 to discuss future directions in high performance computing in Sweden. The meeting started with a presentation by Dick Kaplan from the National Science Foundation (NSF) in the United States. Kaplan has been heavily involved in the evaluation of the proposals for new NSF centers.

This Spring NSF decided to focus their resources on just two centers instead of the four which they had supported during the last 12-year period. Furthermore there will be strong emphasis on cooperation between the NSF centers and local research centers. A smaller fraction of the funding will go to the local partners of the NSF centers. There is also an increase of the emphasis on service, research and development at the centers and their partners and not only the focus on the supply of computing cycles. The new contract is for five years with a possible renewal for another five.

After Kaplan's presentation the implication of the NSF experience on the Swedish situation was discussed. There are large differences in resources but also similarities. It is clear that cooperation within Sweden would be helpful and that a focusing of the limited financial resources mainly on one center will be necessary. Different groups should develop clear profiles to reduce unnecessary overlap. We should also be open to different forms of cooperation between all the Nordic Countries.

In this issue you can find a list of the projects which were granted time in the last round of distribution of computer resources. The number of appli-

cations is still very large and unfortunately many can not be granted time. It seems that the impact from the centers in Göteborg, Linköping and Umeå is not yet being seen. The application process might be a good candidate for cooperation.

Another item in this Newsletter is the report on Deep Blue. There is an interesting spinn-off of that technology. A special purpose processor is being developed by IBM for simulation of multi-particle interactions with applications to astrophysics and molecular dynamics. We shall follow the development and report in later newsletters.

PDCTN is the technology transfer node at PDC and it is sponsored by the European Commission. It recently received approval for three new projects: one dealing with optimal design of fan blades, another the heat control of buildings and the third the simulation of flow in pumps in the paper industry. These projects are sponsored by the Commission and the purpose is to bring the virtues of high performance computing and networking to the European industry. Please contact PDC if you have any suggestions for innovative use of computing in industry. The emphasis should be on application of existing methods or modification of methods rather than development of completely new ones.

Björn Engquist

Director

Ab initio Molecular Dynamics Investigations of Transition Metal Clusters

Henrik Grönbeck, Arne Rosén, Department of Physics, Göteborg University and Chalmers University of Technology,
Wanda Andreoni, IBM Research Division, Zurich

A simple but intriguing question is how physical and chemical properties evolve as atoms aggregate to larger units: From the single atom to the bulk. In what way does the lack of long range order influence materials properties? These are questions which are posed in the field of atomic cluster physics, where an understanding of the size evolution is the general, and long-term goal.

Obviously, the reduced dimensionality results in a discretization of the electronic states, in contrast with the band structure present in bulk samples. Illustrative examples of the electronic quantization, is the marked electronic shell closings observed in electronic properties of simple metal clusters appearing at 2, 8, 20 etc atoms for a monovalent element. In addition to these shell effects of electronic character, some clusters may show size patterns reflecting the geometric configuration. One example of such, geometric shell closings is the enhanced stability of, for example, krypton clusters with icosahedral structure, Kr₁₃, Kr₅₅, Kr₁₄₇ etc.

Computationally, the field of clusters is challenging because of the large scale quantum problem, with an unknown ionic configuration. For clusters, one might expect different structural motifs, and coordinations, than present in the corresponding bulk material. This is, however, an issue which should be addressed from first principles. Model potentials, derived from bulk or surface properties can most likely not account for the rehybridization in these finite system. In our work at PDC, we have applied the density functional formalism [3] using local minimization techniques, and the Car-Parrinello [1,2] method for mole-

cular dynamics, to investigate on the electronic, geometric and chemical properties of small transition metal clusters.

The Car-Parrinello [1] method, is a method to solve the density functional minimization problem, and to perform *ab initio* molecular dynamics. By introducing a fictitious mass for the electrons, the time evolution of a system containing ions and electrons can be studied by solving a coupled set of equations of motion. In this sense, the electrons and the ions are treated in a similar way. The strength of the method has been demonstrated, not only in the field of solid state physics, where it first was introduced, but also for finite systems such as clusters, and molecules [4]. The method uses a plane wave expansion for the electronic wave functions, and pseudo potentials for the description of the inner cores. The use of plane waves is convenient in connection with molecular dynamics, since the calculation of forces does not depend on the atomic positions. Finite systems are conveniently studied without periodic boundary conditions. An embedding geometry is chosen large enough to demand the wavefunctions to vanish at the boundaries. This enable us to perform simulations for charged systems, and processes involving charge exchange. We will below give two examples from our research program at PDC. The calculations were performed using the CP program from IBM [2].

As mentioned above, one intriguing problem in cluster science is the structural configurations. This is an unknown experimental property, and computationally it is difficult due to the large number of possible isomers. We have performed calculations of the

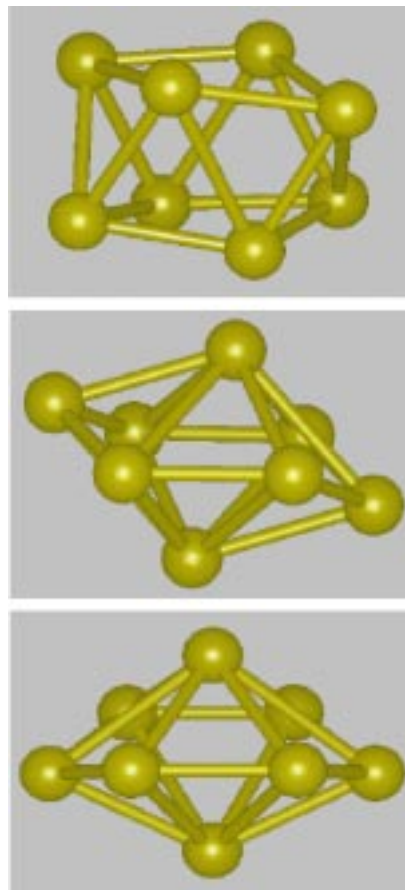


Figure 1
The discussed geometries for Nb₈.

geometric properties of niobium clusters [5]. Niobium is a transition metal, with several interesting features in the size evolution pattern, where the experimental evidence of isomers is one example. For Nb₈, we have by molecular dynamics, and standard geometry optimizations obtained several minima on the energy potential surface. Three of them are shown in Fig. 1. These three isomers are within 0.6 eV in total energy. The lowest energy geometry (top panel) is a dodecahedron, while (mid) and (bottom) both have structures of bi-capped octahedra. All these geometries represent compact structures with a high coordination for all atoms in the cluster.

In addition to bare metal clusters, we have studied the adsorption of molecules such as O₂ and CO onto clusters of niobium and platinum. One example is (CO)_n onto Pt₃. CO on Pt(111) is a school book example of the interaction of CO on transition metal surfaces, which essentially can be understood within the Blyholder model for 5σ donation and 2π backdonation. What happens when the surface is reduced to only three atoms? Is, for example, the same geometric configurations preferred, and what are the characteristic binding energies? In our study, we have found that actually the top configuration is preferred for adsorption of CO on Pt₃, in agreement with CO onto Pt(111). However, the molecular binding energy is much higher (~ 1 eV). For the characterization of CO on surfaces, often the stretch vibration frequency of CO is measured. This has also been done in the case of clusters, using vibrational resolved photo electron spectroscopy (PES) [7]. The vibrations are in this method excited by removing one electron from an anionic cluster. Consequently, it is important where the last electron is localized. We find that for the anion of Pt₃ (CO)₆ that this orbital is delocalized over the entire molecule, Fig. 2. Removing this electron will excite two decoupled vibrations of the top and bridge bon-



Figure 2

Two views of the Pt₃(CO)₆⁻ HOMO probability density. The plotted surface corresponds to 0.001 e/(a.u.)³.

Pt₃(CO)₆ has a planar structure with three CO molecules in top and bridge positions, respectively.

ded CO molecules, respectively. Our evaluation of the vibrational spectrum yields a separation of the top and bridge vibrations, of 173 cm⁻¹, not very different from the surface case.

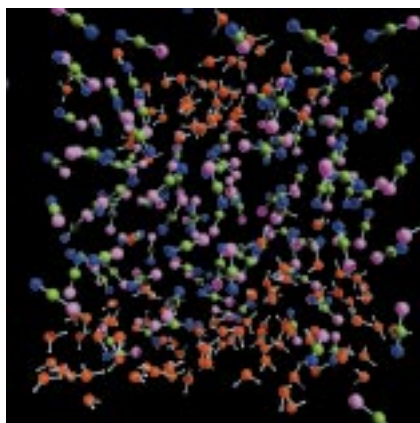
Having taken two examples from our research program, we have demonstrated issues currently of interest in the field of atomic clusters, and some of the possibilities of the methods we are using. The plane wave - pseudo potential method is very powerful in handling dynamical properties of clusters. The application to transition metal clusters, where the

pseudo potentials are hard, and require large cut-off energies is, however, computationally demanding. It is actually thanks to the development of parallel computers and the access to large performance computer facilities that makes investigations of this kind possible.

References

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New SGI Onyx2 at PDC



S GI/Cray has placed an eight processor Onyx2 at PDC for evaluation purpose during six months. The PDC-users may access the machine

A solution of acetonitril in water. The image was created in Rayshade and took about two minutes to render on Boye. The visualization was created by Johan Ihrén and Kai-Mikael Jää-Aro and based on calculations by Aatto Laksonen and Dan Bergman at the Department of Physical Chemistry, Stockholm University.

both for visualization projects or for general purpose computing. The name given to this machine is Boye, following our tradition to name our computers after Swedish authors.

The Onyx2 at PDC contains eight R10000 processors and 2 GB RAM memory. Graphics capabilities are provided by the InfiniteReality system.

The graphics system of the Onyx2 is impressing and we utilized Boye in



several visualization projects and to produce 3D-graphics on the ImmersaDesk. A multimedia installation has also been developed using Boye.

The multi media installation "Digital Runes" by Teresa Wennberg was developed in Alias Wavefront and shown at the Swedish Embassy in Tokyo in April 1997. The final 3D rendering was made on Boye.

News about PDCTTN

The technology transfer node, PDCTTN has signed the contract with DG III. Furthermore, three new activities, SIMMIL, concerning simulation of flow pumps, OPTI-BLADE, studying the design of fan blades and IDASTAR, simulation of heat control in buildings, has been approved. More information will be made available at: <http://www.pdc.kth.se/pdcttn/>.

Current Projects at PDC

Principal Investigator	University	Title	Machine
Andersson Ulf	KTH	Large Scale FDTD	IBM SP, Fujitsu VX/2, Cray J90
Ayani Rassul	KTH	Efficient modeling and simulation of mobile communication systems	IBM SP
Belonoshko Anatoly	UU	Atomistic simulation of high pressure processes in shock waves and diamond anvil cell	IBM SP
Bodare Anders	KTH	Parallel spectral elements for 3D large scale elastodynamics	IBM SP
Bolinder Jonas	LTH	Numerical study of pulsatile developing flow in a curved square duct of strong curvature	IBM SP
Brinck Tore	KTH	Quantum Chemical Studies of Enzyme Catalysis	IBM SP
Broo Anders	CTH	Theoretical studies of molecular device functionality	IBM SP, Fujitsu VX/2
Brorson Mats	LU	PAPP - Programmer's Aid for Parallel Programming	IBM SP
Casanovas Virginie	KTH	Turbulence Modelling for Unsteady Flows in Axial Turbines	IBM SP
Edholm Olle	KTH	Parallel Molecular Dynamics Studies	IBM SP
Ehrenberg Måns	UU	Molecular Control Theory	IBM SP
Eklund Dean R.	KTH	Investigation of the influence of Radiation on Combustor Wall Heating	Fujitsu VX/2
Elofsson Arne	SU	Examination of accuracy of Molecular Dynamics	IBM SP
Elofsson Arne	SU	Development of scientific programs in bioinformatics and protein folding for high-performance computers	IBM SP Fujitsu VX/2, Cray J90
Enwald Hans	CTH	Modelling and numerical simulation of hydrodynamics in fluidized beds	IBM SP
Fransson Torsten	KTH	Aeromechanical Vibrations in Cascades	IBM SP
Fransson Torsten	KTH	Study of Transition in Turbine Cascades and on Wings Using Modern Transition Prediction Methods	IBM SP, Fujitsu VX/2
Grönbeck Henrik	CTH	Ab initio investigation of supported and self-assembled metal clusters	IBM SP
Hallberg Anders	UU	Design and synthesis of protease inhibitors and tumpeptidomimetics	IBM SP
Hermansson Kersti	UU	Water exchange mechanism around Li+	IBM SP
Johansson Arne	KTH	Study of various turbulent flows with direct numerical simulation and LES	Fujitsu VX/2
Jonsell Svante	UU	Resonantly enhanced pion transfer in the cascade of pionic hydrogen	Fujitsu VX/2
Juhlin Christopher	UU	Modeling of seismic waves in 3d heterogeneous media	IBM SP
Kloo Lars	LU	Applied theoretical analyses of inorganic and organometallic cluster systems	IBM SP
Kowalewski Jozef	SU	Nuclear spin relaxation studies	IBM SP
Kropp Wolfgang	CTH	Sound insulation at low frequencies	IBM SP
Laaksonen Aatto	SU	Parallel molecular dynamics simulations of DNA systems	IBM SP
Larsson Karin	UU	Investigations of surface - and gas phase reactions during film growth	IBM SP
Lidmar Jack	KTH	Monte Carlo Simulation of Vortex Dynamics	IBM SP
Lindgren Jan	UU	Ab initio calculations on polymer electrolyte components	IBM SP
Lindh Roland	LU	Ab initio study of the ammonia dimer	IBM SP
Lunell Sten	UU	The ozone depletion problem - DFT study of the ClO self-reaction mechanism	IBM SP
Neretnieks Ivars	KTH	Utveckling av kopplade hydrogeokemiska simuleringsverktyg för paralleldatorer	IBM SP
Nilsson Lennart	KI	Nucleic acid conformational dynamics and protein-nucleic acid interactions	IBM SP
Norberg Jan	KI	Molecular Dynamics Simulations of Nucleic Acids	IBM SP
Oberschmidt David	KTH	First-Principles Calculations of Magnon Spectra and Related Finite Temperature	IBM SP
Odelius Michael	UU	A first principle studie of the dehydroxylation of Muscovite	IBM SP
Peirano Eric	CTH	Numerical solutions of the two -fluid model applied to turbulent gas-solid flows	IBM SP, Fujitsu VX/2
Persson Mats	CTH	Electronic structure calculations for the physics and chemistry of surfaces	IBM SP
Quinteros Teresita	KTH	Elastic light scattering in clusters of irregularly shaped pigments	Fujitsu VX/2
Rein Tobias	DTU	Kvantkemisk undersökning av mekanismen för Horner-Wadsworth-Emmons Reaktion	IBM SP
Rosengren Anders	KTH	Strongly correlated systems	IBM SP
Ryde Ulf	LU	The structure of blue copper proteins studied by theoretical methods	IBM SP
Salomonson Sten	CTH	Two-Photon QED Corrections in Highly-Charged Ions	IBM SP
Sarman Sten	CTH	Molecular dynamics of liquid crystals	IBM SP
Sten Lunell	UU	Quantum chemical studies of surface reactions on titanium dioxide	IBM SP
Svensson Mats	KTH	An MO-MM approach for studying Transition Metal Catalyzed Reactions	IBM SP
Szabo Kalman	UU	Computational Studies on Electronic and Steric Interactions Governing the Selectivity in Transition	IBM SP
Thomas Josh	UU	MD Simulation of Ion motion in polymer surfaces and polymer electrode interfaces	IBM SP
Widmalm Göran	SU	Carbohydrate dynamics	IBM SP

Calendar of Events

August

- 18-29 **PDC Summer School 97**
Introduction to HPC.
PDC, KTH, Stockholm
<http://www.pdc.kth.se/training/training.html>
- 18-20 SCAI '97
Sixth Scandinavian Conference On Artificial Intelligence
Helsinki, Finland, August 18-20, 1997
<http://www.cs.helsinki.fi/events/SCAI97/>
- 22-24 15th IMACS World Congress 1997 on Scientific Computation, Modelling and Applied Mathematics
Berlin, Germany
<http://www.first.gmd.de/imacs97/>
- 26-29 Euro-Par'97
Passau, Bavaria, Germany
<http://brahms.fmi.uni-passau.de/cl/europar97/>

September

- 1-3 First European Conference on Research and Advanced Technology for Digital Libraries
Pisa, Italy
<http://www.area.pi.cnr.it/ErcimDL/dl3.html>
- 4-8 EUROGRAPHICS '97
Budapest, Hungary
<http://www.sztaki.hu/conferences/eg97/>
- 10-12 Computer Science for the Environment '97
1st European Conference on Information Technologies for the Environment
Strassbourg, France
<http://www.inria.fr/Colloques/ENVIRONNEMENT-eng.html>
- 11-12 Third European CRAY-SGI MPP workshop
Paris, France
<http://www.cea.fr/workshop>
- 16-19 ParCo97
Parallel Computing Conference
Bonn, Germany
<http://www.gmd.de/SCAI/parco97>
- 24-26 WDAG '97
11th International Workshop on Distributed Algorithms
Saarbrücken, Germany
<http://www.mpi-sb.mpg.de/~wdag97>

October

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

- 19-23 ESS'97, 9th European Simulation Symposium and Exhibition
Passau, Germany
<http://hobbes.rug.ac.be/~scs/conf/ess97/>
- 28-29 SP2 World '97 (former Sup'Eur)
Egham, UK

November

- 5-8 HiPer' 97 High Performance Computing on Hewlett-Packard Systems
Krakow, Poland
<http://www.cyf-kr.edu.pl/hiper97/>
- 15-21 SC97: High Performance Networking and Computing
San Jose, CA, USA
<http://scxy.tc.cornell.edu/sc97/>
- 22-29 SOFSEM '97, XXIV-th Seminar on Current Trends in Theory and Practice of Informatics
Milovy, Czech Republic
<http://www.ics.muni.cz/sofsem/sofsem.html>

December

- 18-19 **PDC Conference**
PDC, KTH, Stockholm
<http://www.pdc.kth.se/news/events/events.html>

Software overview

There has been some changes and updates of the software at PDC. This table offers an overview of the current version of some of the software at PDC.

	IBM SP	Fujitsu	Cray	Other
Physics/Chemistry				
Gaussian-94	E.2	E.2	E.2	
GAMESS	Jan-97			
MacroModel/BatchMin	5.5			
CHARMM	25a1			
Solid Mechanics				
ABAQUS/Standard	5.5par		5.6-1	Nyx
ABAQUS/Explicit			5.6-1	
Video software				
SpeedRazor				PC
Alias/Wavefront				Boye
NAG libraries				
f77-library	17			
f90-library	2			
MPI-library	1			
NAGware products				
f77-tools	2			
f90-tools	2			
Numerical libraries				
MASS	2.3			
BLAS		REF		
BLACS/PBLAS	REF			
ARPACK	-96	-96		
PARPACK	-96			
LAPACK	2.0	2.0		
Productivity tools				
Matlab	5.0		4.11	Boye, Nyx



Deep Blue Wins Over Kasparov

Carl G Tengwall from IBM followed the game. Here is his report from the match.

Newsweek called it "The Brain's Last Stand". To computer scientist the problem of making computers play strong chess has been a challenge for nearly half a century. In the beginning of May, Garry Kasparov and Deep Blue squared off in their rematch. Last year Kasparov, after what most people considered an embarrassing loss of the first game, went on to win the encounter by 4-2.

This year the team from IBM T.J.Watson Research Laboratory in Yorktown Heights saw their Deep Blue computer win its rematch against the reigning chess world champion. Deep Blue is a 32 node IBM RS/6000 SP computer. Each node has two boards with eight chips that have been custom built to generate and evaluate chess positions at a high rate. The 32x2x8 = 512 chips working with the regular SP processors were able to evaluate more than 200,000,000 chess positions per second. Apart from a factor of two increase in processing speed Deep Blue this year had stronger tools for playing the opening (a complete book of published games between grandmasters), enhancements in the evaluation function that allowed it to play a much stronger middle game, and finally Ken Thompson's book of end games with five pieces or less. The Deep Blue team, under the leadership of IBM's C.J. Tan, had also enlisted the help of chess grandmaster Joel Benjamin, former US chess champion.

That Benjamin's preparations were effective was demonstrated particularly in Game 2. The way the computer handled the closed position by time and again shifting the play from the King side to the Queen side and back, clearly impressed everyone, Kasparov included. In Game 5 the computer managed to draw a position that Kasparov probably was quite certain he would win. It was in some sense logical that the final game (No. 6) of the match ended after just 19 moves. Garry Kasparov had actually committed a serious opening error that allowed the computer a very strong sacrifice already in move eight. The final score was a win for Deep Blue by 3.5 - 2.5.

We will not know until later what will happen in the computer chess area, but IBM is busy investigating similar cost-effective hybrid technologies such as Deep Blue for other tasks. Among those mentioned are Molecular Dynamics, Financial Risk Assessment and Data Mining.

See <http://www.chess.ibm.com/> for more information.

New Version of Kerberos

We have upgraded the Kerberos server at PDC. If you have a version of the Kerberos travelkit older than version 0.9.5 you might want to upgrade. The upgrade does not affect all the programs in the travelkit, older versions of telnet and kauth are still compatible, but an older ftp will not work. Binaries for the most popular versions of UNIX are available at our website, see <http://www.pdc.kth.se/support/kerberos-tour.html> for more information on how to download and install the travelkit. Source code can also be found for various operating systems at our web. Contact PDC if you have any problems with Kerberos.

Protecting your data and computers against malicious attacks is today a necessity. At PDC we use Kerberos to offer secure access to the computers. The Kerberos system is named after the three headed dog who guards Hades in Greek mythology. Incidentally, a statue of Kerberos can be found at the KTH campus just outside PDC. The Kerberos software was developed at MIT. Currently, version 5 is under development, version 4 is being used at PDC.

Kerberos works by issuing tickets and secret cryptographic keys to the user. These tickets are then used to identify the user towards computers and services in a networked environment. In order to prevent replay attacks, where an attacker listens to network traffic and later try to replay an authentication, a timestamp is provided with the ticket. If a ticket is too old, it won't be valid. Your local workstation clock must be in sync (within a few minutes) with the machine you are communicating with or else your tickets will be treated as non valid. The cryptographic key should prevent eavesdropping and the timestamp should stop replay attacks.

The idea is that by knowing your password you can get a ticket and a key to prove your identity. A ticket is however valid only once, so for each new authentication you need a new ticket. To have to enter your password every time you need a service at the host, would be a very tedious process. The obvious solution, to cache the user's password locally has some drawbacks. Instead, Kerberos issues a special ticket when you log in, a "ticket granting ticket" with a lifetime of eight hours. This ticket granting ticket is then used to issue new tickets. One problem we see is that when you submit a long job, or a job that spends a long time in the queue, your ticket granting ticket may have expired when the job has finished. This means that saving results from that run will not be permitted by the system. Avoid this problem by using `kauth -l<time>` when submitting a job that will not finish in less than eight hours. The time should be given in minutes, `kauth -l 4500` would give me a ticket valid for approximately three days.

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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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