PDC Newsletter

Gaussian Creator Wins Nobel Prize

The 1998 Nobel Prize in Chemistry

the work of
Professor Walter Kohn
Professor John A. Pople

presented by
Professor Björn Roos
Member, The Swedish Academy of Sciences; Member, The Nobel Committee for Chemistry

PRIZE CITATION: (Kohn) "for his development of the density-functional theory"

PRIZE CITATION: (Pople) "for his development of computational methods in quantum chemistry"

EDITOR'S NOTE: *The computer program Gaussian, for which John Pople received the Nobel Prize in Chemistry, is the most general computational chemistry software package in use today, and it is the most-used computational chemistry software package at PDC.*

British citizen John A. Pople of Northwestern University, in Chicago, Illinois, receives his prize in chemistry from King Carl XVI Gustaf of Sweden at the Nobel Award Ceremony at the Concert Hall in Stockholm on December 10,1998.
PHOTOGRAPH: COPYRIGHT ANDERS WIKLUND, SCANPIX.

"Your Majesties, Your Royal Highness, Ladies and Gentlemen,

Man is fantastic. Through his studies of nature, he has brought order to chaos. He has created a language, mathematics, which makes it possible to formulate his knowledge about nature in a small number of simple sentences. Not only do these sentences summarize in a concentrated manner our knowledge about nature and matter, they can also be used to make predictions. With the aid of computer simulations, we can make weather forecasts, calculate the structural integrity of bridges, the aerodynamical characteristics of airplanes, etc. Today, we celebrate the fact that mathematics has invaded chemistry, that by means of theoretical calculations we can predict a large variety of chemical phenomena. Professors Walter Kohn and John Pople have individ-

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ually made fundamental contributions to this development.

An atom consists of a nucleus and electrons. The motion of the electrons is described by the laws of quantum mechanics. When these laws were formulated more than 70 years ago, researchers realized immediately that in them was contained the explanation of the che-mical bond. It was realized that if the quantum mecha-nical equations could be solved, one would be able to explain how atoms are bound together to form molecules. It would be possible to ex-plain why molecules look as they do, what their properties are, and how they react with each other to form new molecules. A theoretical description of all of chemistry was within reach.

To achieve all this was, however, not easy. The equations are complicated, and in the beginning it was only possible to solve them for the simplest cases. The science of applying quantum mechanics to chemical phenomena therefore developed only slowly. It was only in the beginning of the '60s, when scientists could start using computers, that this development started to make rapid progress. John Pople was one of the scientists who understood at an early stage the potential that computers provided. He realized that if quantum chemistry was going to become important in chemistry, one had to develop methods which were effective and which could be used to compute interesting properties like the structure of molecules and binding energies for the chemical bonds. They also had to be easy to use for the general chemist, who could not be expected to be knowledgeable about all the subtle details of quantum chemistry. Pople was able to fulfill these conditions through a series of crucial innovations and improvements. He designed a new tool, which could be used to study molecules and compute their properties. This tool is a computer program called Gaussian. It contains a theoretical model chemistry where quantum mechanical equations are solved through a series of more and more refined approximations. Pople's methods are used today by thousands of scientists at universities and companies around the world to study a large variety of problems in chemistry and biochemistry.

The methods that John Pople has developed seek approximative solutions to quantum mechanical equations, where the fundamental quantity is the so-called wave function, which describes the motion of all electrons. In two landmark articles from 1964 and 1965, Walter Kohn showed an alternative way in which quantum mechanical equations can be approximated. He showed that there is a one-to-one correspondence between the energy of a quantum mechanical system and its electron density, which is a function of three positional coordinates only and is, therefore, much easier to handle than the complicated wave function, which depends on the positions of all electrons. He also developed a method that made it possible to construct a set of equations, which could be used to determine the energy and electron density. This approach, called density functional theory, has developed during the last ten years into a versatile computational tool with many applications in chemistry. Due to its simplicity, it can be applied to larger molecules than the wave-function-based methods. Density functional theory has made it possible to study the mechanisms of chemical reactions in enzymes, for example, when water is transformed into oxygen in photosynthesis.

Due to extraordinary circumstances, Professor Walter Kohn is not with us today. We hope to see him at the Prize Ceremony next year, instead.

Professor John Pople,

I have tried to describe in a few words how Professor Kohn's and your work has led to a new revolution in chemistry. You have made fundamental contributions to the field of quantum chemistry, with the result that chemists and biochemists today have a new tool, which they can use to study chemical phenomena at a molecular level. This is an outstanding achievement. On behalf of the Royal Swedish Academy of Sciences, I wish to convey to you our warmest congratulations, and I now ask you to receive the Prize from the hands of His Majesty the King ”

From the Editor

The research behind the Nobel Prizes relies increasingly on high-performance computing. It was an essential component in the work of Kenneth Wilson, who received the 1982 Nobel Prize in Physics.

The latest Nobel Prize in Chemistry exemplifies yet another step in the recognition of scientific computing. John Pople was awarded "for his development of computational methods in quantum chemistry." The focus is thus on the actual development of the computational technique, and not only on the results derived from the computations.

The program Gaussian, developed by Pople and his coworkers, is one of the most frequently used codes at PDC. Starting later this year, we plan to work on its implementation on the new SMP nodes in order to achieve higher efficiency.

It is clear that in modern science, computing often has the same importance as the classical tools of theory and experimentation. Scientific computing frequently provides the only practical link between theory and experimentation. Modern theories are formulated using advanced mathematics, and a high-performance computation is very often the only way to produce quantitative results from these mathematical models, which can then be compared and verified with experiments.

When a mathematical model and its related computer program are well verified, the computer can act as a virtual laboratory. This is possible in fundamental physics and chemistry, as well as in the engineering sciences; for example, a direct Navier-Stokes solver can be used to derive and analyze turbulence models.

On the organizational side of PDC, several academic computing centers in Sweden plan to create a joint program committee that will streamline the processes of applying for and allocating computing resources. We will build on our recent experiences from coordinating the application process with HPC2N and NSC. Our hope is to have the new processes in place before the upcoming summer.

Finally, I would like to welcome the new members of the PDC board. Kersti Hermansson from the chemistry department of Uppsala University has been a valuable member of the PDC Science Council in the past, and her background in chemistry will certainly be an asset to PDC and all its users in the field of computational chemistry. Anders Eriksson, the new Prorektor at KTH, not only represents the Royal Institute of Technology but also contributes by virtue of his experience as previous director of the Kallsup project and from his own research using engineering computing. Hans Wallberg is the director of UMDAC, and he is also responsible for coordination and development of SUNET and thus the ideal representative for the increasingly important N (networking) in HPCN. He also has valuable experience from his time as a board member of HPDR.

These three members join the four returning members of the board. We are confident in their extremely valuable combined experience, and we look forward to working together with them.

Björn Engquist
Director

Education on line

On-line training and educational materials are available through the PDC Web site at <**http://www.pdc.kth.se/training/**>. These materials include *Parallel Programming and Programming Languages*, *SMP Programming for the IBM SP*, and *Parallel Environment and Tools on the IBM SP*.

Correction

All of the photographs of the VR-CUBE in Volume 3, No. 3, of the PDC Newsletter (Autumn 1998) were taken by Thomas Asplund of KTH. We regret this credit omission.

PDC Board

New members

Anders Eriksson
Institutionen för byggkonstruktion
KTH (prorektor)

Kersti Hermansson
Ångströmlaboratoriet
Uppsala universitet

Hans Wallberg
UMDAC
Umeå universitet

Returning members

P.G. Hedström
Electrolux AB

Gunnar von Heijne
Biokemi
Stockholms universitet

Anne-Marie Pilotti
Teknikvetenskapliga forskningsrådet

Gustaf Söderlind
Datalogi och numerisk analys
Lunds universitet

Theoretical Studies of Biochemical Reaction Mechanisms

Margareta Blomberg and Per Siegbahn
Department of Physics, Stockholm University

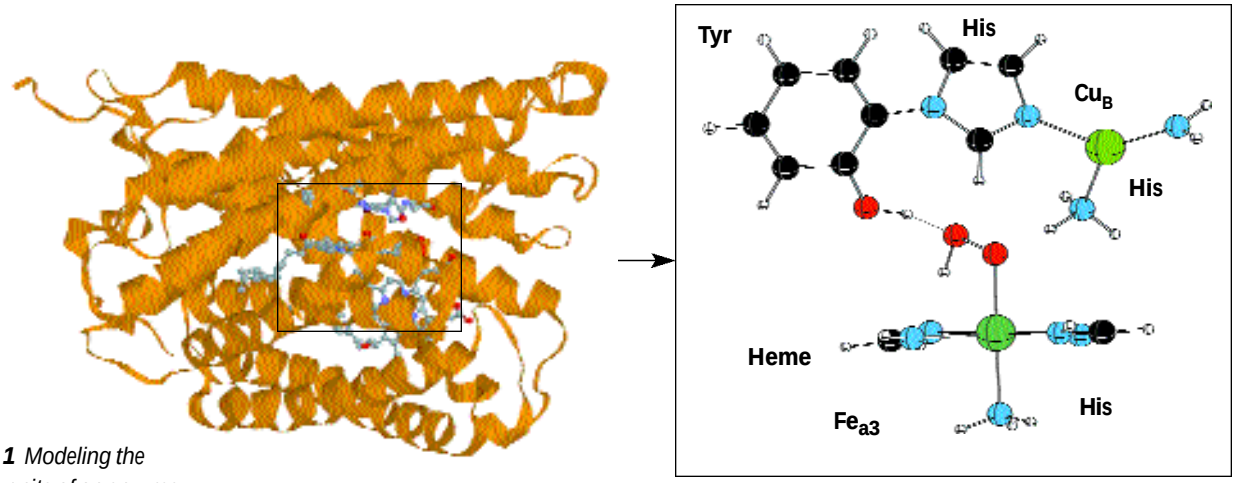


Fig. 1 *Modeling the active site of an enzyme*

Part of CcO (Unit I)

Binuclear Center

Some twenty years ago, quantum chemistry could only be used to study the properties of very small molecules, for example, spectra of diatomic molecules or the relative energies of different isomers of small organic molecules. The dramatic development of computational methods in quantum chemistry during the last twenty to thirty years, which rewarded Walter Kohn and John Pople with the 1998 Nobel Prize in Chemistry, has made it possible to study more interesting aspects of chemistry and chemical reactions. In particular, the development of density functional theory, initiated by Walter Kohn, allows for accurate and extensive investigations of systems as large as 50-60 atoms. Because of the Gaussian program package, begun by John Pople, researchers can take advantage of the most recent quantum chemistry developments. Our group is using these new opportunities to study mechanisms of biochemical reactions, in particular those of metallo-enzymes. We use the hybrid density functional method B3LYP – which contains Hartree-Fock exchange and only a few (three) empirical parameters – to calculate reaction energies and activation energies for models of the active sites in metallo-enzymes. Below we describe some examples where the Gaussian 94 program is being used.

One of our major projects concerns the mechanisms for the photosynthetic water oxidation in green plants. This reaction takes place at a manganese cluster, and our calculations on model manganese complexes give thermodynamic support for a recently suggested mechanism in which a tyrosyl radical abstracts hydrogen atoms from the water molecules. The last step in the water oxidation, during which the oxygen molecule is formed, is the most difficult one to describe, in part because the structure of the manganese cluster is not known. After thousands of calculations on different model systems, containing up to 42 atoms, a mechanism for the O_2 formation is emerging. This mechanism involves the formation of an oxygen radical, which was not previously suggested.

We are also studying the mechanisms for the reverse reaction – the reduction of molecular oxygen to water – that occurs in the respiratory chain. This reaction takes place at an iron porphyrin and involves a nearby copper-histidine complex. Using a 50-atom model of

this binuclear center, which is situated in the cytochrome c oxidase enzyme (see fig. 1), we are investigating different mechanisms for the O_2 activation reaction. Our calculations suggest a mechanism for how the energy released in the O_2 reduction is used to pump protons across the membrane, which ultimately results in ATP production.

Another part of photosynthesis is the charge-separation reactions and electron-transfer reactions, which are driven by light, that occur in the chlorophyll chromophores. Our model calculations agree with experimentally known results for bacterial photosynthetic reaction centers, and they also indicate some structural differences between the bacterial and plant reaction centers. For charge-separation reactions, the stabilizing effects of the surrounding protein have to be taken into account. This is done in our calculations by treating the protein as a homogenous low-dielectric medium, using the SCI-PCM method as implemented in the Gaussian 94 program. The largest individual system treated in these charge-separation calculations is the 92-atom model of the special pair of chlorophylls in the bacterial reaction center (see fig. 2).

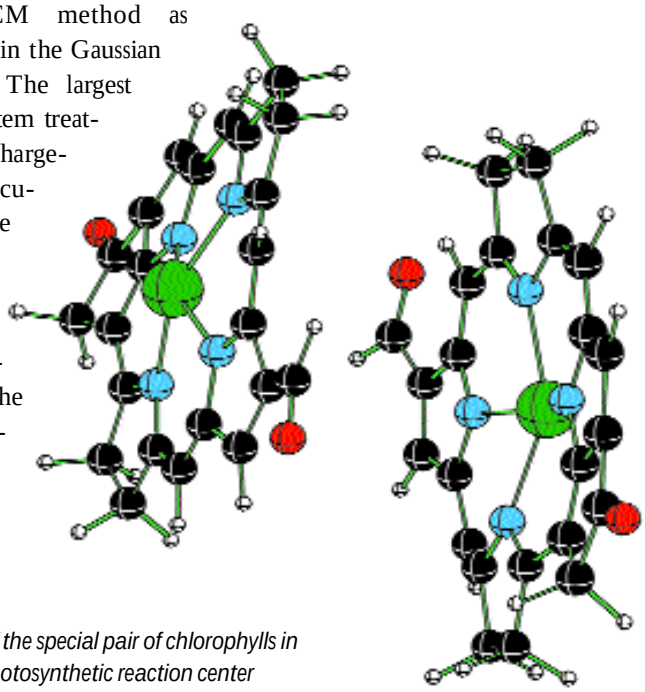


Fig. 2 *Model of the special pair of chlorophylls in the bacterial photosynthetic reaction center*

PDC Upgrades

PDC has begun the first of two upgrades to its IBM RS/6000 SP supercomputer in 1999. The upgrades will allow users' jobs to run faster, and to use more memory and more disk space. Users will also be able to take advantage of new features of the operating system and parallel computing environment. These include user-initiated checkpointing, and the ability to run multiple jobs using the high-speed user-space protocol. The upgrades also allow PDC to introduce a new service that will provide the possibility of a permanent global file space for researchers' projects.

The two upgrades will boost the performance of PDC's IBM SP with the acquisition of additional symmetric multiprocessors (SMPs). SMPs, which consist of multiple CPUs on the same node, are now playing the role of the computational element in scalable distributed memory systems like the IBM SP. An increase in the number and speed of CPUs in SMPs – as will occur in these upgrades – has the potential to multiply the performance of programs that can make use of the added level of parallelism.

On the hardware side, PDC will add sixteen new IBM symmetric multiprocessor 604e-based PowerPC nodes to the current IBM SP configuration. Each PowerPC node has four processors, which brings the total number of additional CPUs to sixty-four. During the second upgrade, four new POWER3 nodes, each carrying eight CPUs, will be added. The result of these upgrades is summarized in the table above.

	Nodes	*CPUs*	*Peak GFLOPS*	*RAM GB*	*Local Disk GB*	*Global File System GB*
Current:	154	172	104	51	730	128
After 1st upgrade:	170	236	148	71	920	256
After 2nd upgrade:	174	268	173	87	1064	256

On the software side, PDC will upgrade the IBM SP's operating system to AIX 4.3.2, the parallel system support program to PSSP 3.1, and the parallel environment for AIX to PE 2.4. These fundamental changes to the system should result in an even more stable environment for programs, and one in which multiple programs can run in high-speed "user space." PDC will also replace the parallel file system (PFS) with the general-purpose file system, GPFS. Not only does GPFS provide more stability and speed than PFS, but it also has the capacity for backup as well. As a new service, PDC will offer the placement of projects in a permanent location in GPFS.

To help users leverage this new environment, PDC will offer a two-day course in symmetric multiprogramming (SMP), May 11-12.

Details about the PDC upgrade, including the current status, can be found at
<http://www.pdc.kth.se/sp/>

The exact date, location, and registration form for the SMP courses, will be at
<http://www.pdc.kth.se/training/1999/SMP/>

Future Directions in Visualization

Greg Johnson, Dave Pape, Tom DeFanti, Rachael Brady, Ulrich Lang, and Thomas Reuding discuss their ideas about the future of visualization and virtual reality with audience members during the panel discussion at the 1998 PDC annual conference.

Eight invited speakers – from Sweden, Germany, and the United States – came to PDC's annual conference to discuss current trends in visualization, as well as future directions of this technology.

Conference participants were invited to experience for themselves the PDC VR-CUBE, the world's first fully immersive, six-surface visualization environment.

The speakers covered a wide range of topics in their individual presentations, including collaborative visualization, tele-immersion, and virtual prototyping environments. Other talks focused on trends in imaging science, virtual environment applications, and the use of VR to gain insight. They discussed the application of VR in fields as varied as health care, car manufacturing, weather prediction, and narrative art.

There was a consensus among the speakers that VR is becoming an increasingly important tool for scientific visualization, and that back-projected immersive technologies are currently a better way to facilitate scientific insight than other methods of VR, such as head-mounted displays.

A lively panel discussion, "The Future of VR Technology," gave audience and panel members an opportunity to interact as a group. They touched on everything from practical questions, such as the usability of new plasma display walls, to speculative issues, such as the types of VR rides Disney might produce in the future.

The presentation abstracts from the conference are available on line at **<http://www.pdc.kth.se/news/events/conference98/>**

Calendar of Events

General

March

30–April 4 SOLAR'99 (5th International Conference) and ENPHO'99 (2d International Training Workshop); Cairo, Egypt
http://www.photoenergy.org/solar99.html

April

12–16 2d Merged Symposium IPPS/SPDP 1999:13th International Parallel Processing Symposium & 10th Symposium on Parallel and Distributed Processing; San Juan, Puerto Rico
http://www.ippsxx.org/ipps99/

13–15 5th European Conference on Electrochemical Processing; Chester, England
http://www.etbusiness.com

19–21 Annual Meeting of the Parallel Tools Consortium (Ptools'99); Boulder, Colorado

May

3-4 3d Symposium on Analysis of Peptides; Stockholm, Sweden
http://www.swepharm.se/

4–7 5th Asian Conference on Analytical Sciences (ASIANALYSIS V); Xiamen, China
http://www.xmu.edu.cn/sedc/english/confer.htm

5 6th Workshop on I/O in Parallel and Distributed Systems (IOPADS); Atlanta, Georgia
http://www.cs.dartmouth.edu/iopads

23–26 Parallel CFD 99; Williamsburg, Virginia
http://www.parcfd.org/1999conf/

June

2–6 2d Workshop on Large-Scale Scientific Computation; Sozopol, Bulgaria
http://orca.st.usm.edu/~marcin/mp/cfp/SciCom99.html

PDC Events

Workshop

SMP Programming for IBM RS/6000 SP Systems; May 11-12

NGSSC Summer School

Introduction to High-Performance Computing; August 16-27

Annual Conference

Simulation and Visualization on the Grid; December 15-17

README

- **OpenMP – C/C++** The OpenMP standard for directives to compilers for shared memory parallel machines has been released in a C/C++ version. This document and the earlier Fortran standard are available at <**http://www.openmp.org/**>.
- **E-mail forwarding** Users are kindly reminded that they should arrange for their e-mail at PDC to be forwarded to an e-mail address of their convenience. This is done by creating the file **$HOME/Public/.forward**, which contains the e-mail address to which your mail will be forwarded. You also need to create a link to this file from your home directory, by using the `ln -s Public/.forward $HOME` command.

Read more at <**http://www.pdc.kth.se/support/ tours.html**>, under "Misc. tours."

- **Is your project time expiring?** To check if your project is expiring, use the `cac examine` command. If your project has expired, your jobs will be overtaken in the job queue by other jobs that have allocated project time. Try, for example, `cac members $USER` followed by `cac examine op143` to check your allowed CACs and their status. Also available is the `cac help` command.

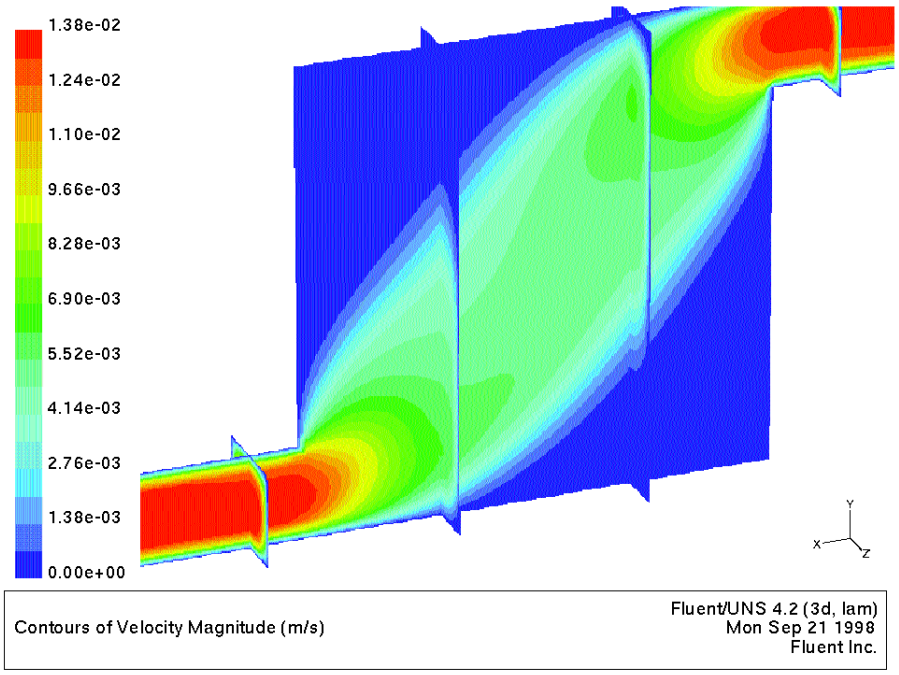
SIMMILL

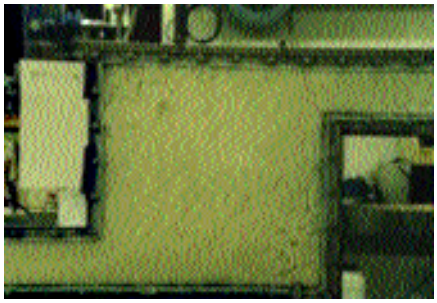
The physical cause of the ketchup effect ("first nothing, then nothing, then everything") is non-Newtonian rheological behaviour. Put simply, the fluid in question does not behave like water. In modern processing industries, such as pulp and food industries,non-Newtonian fluids pose a difficult problem.

When cellulose pulp is transported in pipe and tank systems, problems can appear that depend on the fibre and water content. With a fibre concentration of ten percent, the pulp is a thick suspension. Production in a mill can be interrupted by stationary flow regions within a tank or a vessel. Until now, stop-gap solutions have come from manual experimentation. Massive investments of time and personnel are required to conduct experiments while maintaining maximum capacity operation of a production facility.

However, help is a hand. Kværner Pulping,AB;Prosolvia (technical consultants in the area of computational fluid dynamics); and PDC have worked together to create a computer model to study and optimise flow patterns for the transport of pulp. The results of SIMMILL (Simulation Pulp Mill) are applicable to a number of other industrial processes involving the transport of non-Newtonian fluids. SIMMILL gives quantitatively good results in simulations on real production processes.Kværner Pulping forecasts that the cost and time for the development of process equipment can be reduced by up to forty percent.

Such modelling has become possible and economically feasible through the use of parallel computers. Parallel computer modelling decreases simulation times and costs. This modelling shows that the simulation of non-Newtonian liquid flow and characteristics during transport can be used to adapt and optimise the design and construction of equipment for many types of industrial processes.





Velocity contours, in meters per second, for 10% pulp flow – from a non-Newtonian flow simulation (viscosity model: Herschel-Bulkley). Red indicates faster flow, and green and blue indicate slower flow. Note the stagnant flow in the corner regions, which is typical of high- and medium-consistency pulp.

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

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