NSC News
National Supercomputer Centre at Linköpings universitet
2008:1

Making History

Our first supercomputer is now on display at the National Museum of Science and Technology in Stockholm.

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Electron Transport

Yi Luo is using NSC systems to study electron transport in single molecules and nanostructures.

Read further on page 3

Many thanks to Sven – Welcome to Bengt

Sven Stafström

Bengt Persson

In the last issue of NSC News Sven Stafström told that he was about to leave his position as director of NSC. As he said, it was time to move on in his career. Sad for us, but good for the Department of Science and Technology (ITN) at Campus Norrköping of LiU where he is its new chairman since the beginning of this year. No surprise that Sven was offered this important position. During his four years at NSC he has shown fine leadership by his ability to structure and plan activities and to take strategic decisions. Moreover he has contributed strongly to the team spirit among all the persons at NSC. By open door policy and presence!

During Sven's directorship NSC has moved forwards in important ways. In addition to the support to academic users – which has been maintained on a high professional level – collaborations with external partners, for example SMHI, have been strengthened. A great leap forward, is, of course, Neolith, the 23:rd fastest supercomputer in the world when installed in the new computer hall last fall. Many thanks, Sven, for your input to all of this and more.

Bengt Persson, the new director of NSC, is professor of Bioinformatics at Theory and Modeling at IFM, Linköping University. He and his research group are also affiliated with Karolinska Institutet in Stockholm. His research focuses on biostructural simulations with homology modeling, molecular dynamics and large-scale sequence comparisons. He is also principal investigator for the Biogrid project within the Nordic Data Grid Facility (NDGF). His research profile is evidently computationally intensive with high demands on compute power, data bases and access to high-capacity networks. His strong focus on "bio" is most welcome at NSC and so is Bengt.

KARL-FREDRIK BERGGREN
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The Guide to the Infrastructure

In December 2007, the second version of the roadmap for research infrastructure was finished. It describes current and planned infrastructure of importance for Swedish research, including Swedish efforts in the light of the ESFRI projects (European Strategy Forum for Research Infrastructure). Apart from the planned European large-scale high-performance computing project PRACE, the roadmap covers strategies within physics, astronomy, biosciences, material sciences and further disciplines. A version in Swedish is available via the homepage of VR, the Swedish Research council, http://www.vr.se, and an English version is in preparation.

A New Swedish HPC Landscape

SNIC is currently working on the new version of the Swedish HPC Landscape Document. This strategy document will cover the period from 2008 to 2011. Fundamental changes can be foreseen, such as increased grid computing, growing importance of large-scale storage solutions, international collaborations, and arrival of the first test systems for petaflop computers. Many more things will also be covered, and NSC welcomes input during the writing of this document.

New staff member

Hello everyone! My name is Thomas Bellman, and I'm new here at NSC, so please be gentle with me. I will be working with systems administration, with a focus on grid systems and grid storage. In my previous lives, I have worked in the industry as a programmer, making database systems and internet firewalls.

Electron Transport in Single Molecul

Electron transport is an important process that controls physical properties and chemical activities of many molecular and biological systems. Many applications, such as biosensors, solar energy, molecular and bioelectronics, just to name a few, have been greatly benefited from the good understanding of various electron transport phenomena involved. The study of electron transport in single molecules is also driven by the ever-growing demand for miniaturization of electronic components. Single molecular electronic devices are considered to be the ultimate solution for future information technology. Great progresses have been achieved over the past decade in making various functional devices with electron tunneling, rectification, negative differential resistance (NDR), and switching behavior. However, the underlying mechanisms of these behaviors are not always well understood due to lack of detailed information about the molecular conformations and molecule-metal contacts. The actual existence of molecules inside the devices was even the subject of discussion. Finding molecular fingerprints in molecular junctions has become one of the key issues in the field.

We have developed a quantum chemical approach for modeling electron transport in molecular junctions and implemented it into our own program package QCME (quantum chemistry for molecular electronics)[1]. The method is based on scattering theory and allows to treat both elastic and inelastic electron tunneling on equal footing. It is a bottom-up approach that differs from the traditional solid-state top-down approaches. The use of modern quantum chemistry methods enables us to provide accurate description for molecular systems. More importantly, it allows to effectively studying the effect of intra- and inter-molecular interaction on electron transport.

The first example is the modeling of inelastic electron tunneling spectroscopy (IETS) of molecular junctions, which is a result of electron-vibration coupling in electron transport process.

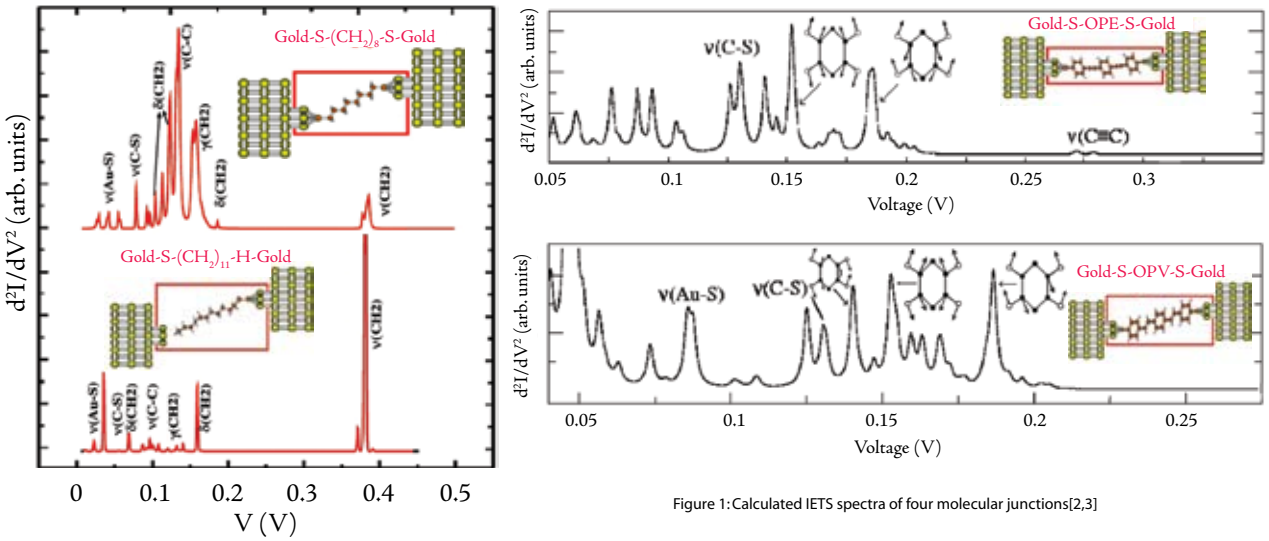

Figure 1: Calculated IETS spectra of four molecular junctions[2,3]

The Story of Cray Number Nine

The Cray-1 supercomputer, legendary for innovative technology and striking design, was introduced in 1975 by the equally legendary Seymour Cray. At that time the Cray-1 meant a great leap forward in computing power and was therefore referred to as "super". The Cray-1 with serial number 09, i.e. one of the first "supers" and Sweden's first, is now on permanent display at the National Museum of Science and Technology (Tekniska museet) in Stockholm. The Cray-1 delivered 160 megaflops, at that time a tremendous performance. Today that is, as we all know, history. To have "our" Cray-1 in the collection of all other remarkable computers at the museum in Stockholm is, however, thrilling. Because it is not just any "super" – to have a Cray-1 in the collection is as prestigious as showing a Spitfire fighter air plane at an aerospace museum. Today there are very few Cray-1 computers left in the world and we are talking about no. 09!

This Cray system was initially purchased in 1976 by the European Centre for Medium-Range Weather Forecasts, Reading, UK, of which Sweden is a member. Getting access to a compu-

es and Nanostructures

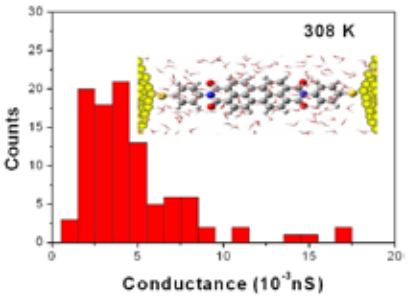

Figure 2: Histogram of conductance of a molecular junction.

A good description of IETS could thus provide detailed information about molecular conformation and molecule-metal bonding in molecular junctions. Figure 1 shows calculated IETS spectra of four molecules sandwiched between two gold electrodes, which are in excellent agreement with their experimental counterparts[2,3]. Calculations indicate that the chemically bonded alkan-chain remains planar while the physically adsorbed specie is twisted inside the junctions. Molecular OPV and OPE are found to be loosely bonded with metal electrodes. We have also demonstrated in other studies how to use IETS to identify intermolecular interaction and the switching mechanisms in molecular junctions.

Many junctions are made in solutions. How the inter-molecular interaction or solvents affect electron transport in molecular junctions has become an important issue. We have developed a hybrid method that combines molecular dynamics simulations with quantum chemical calculations to describe the statistical behavior of molecular conductance. The obtained histogram of conductance, as shown in Figure 2, provides a realistic representation of experimental data. It is also clearly demonstrated that the distribution of molecular conductance can not be described by a simple Gaussian profile used in the statistical analysis of experimental data.

Another dynamic behavior that we have dealt with is the motion of metal ion in fullerenes. We have found that for a series of endohedral metallofullerenes the metal ion can oscillate around its equilibrium position on a flat potential energy surface, see Figure 3. The amplitude of the oscillation increases with the increase of the temperature and can be determined by near-edge X-ray absorption spectroscopy[4]. We have also found that the dynamic motion of metal ion inside the cage can result in very different electron transport behavior depending on the locations of the electrodes, which is a unique property that could be used to make functional metallofullerene devices.

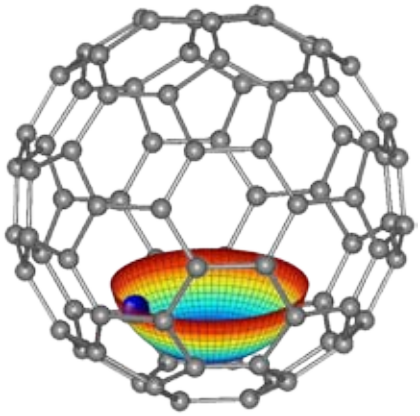
Figure 3: Potential surface of a metal ion oscillating around its equilibrium.

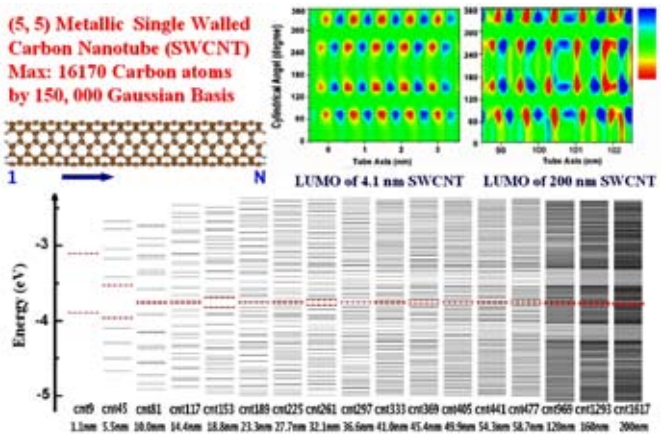

Figure 4: Calculated electronic structures of (5,5) SWCNTs of different length.

Elastic electron tunneling is often a dominant process in molecules of small size. Its domination is believed to be diminished when the size of the molecule gets larger. However,

ter of this kind meant a new era for weather forecasting. All of this has now evolved into a grand art including also climate modelling.

After seven years at Reading, number 09 was sold in 1983 to Saab Aircraft in Linköping for 30 MSEK. At Saab it was used for heavy computations in solid mechanics and aerodynamics when developing the JAS 39 Gripen fighter. The Cray-1 was an absolute necessity for completing such studies in time. However, the Cray-1 offered more than that. Thus Saab and the Swedish Natural Science Research Council signed a long term agreement that the computer could also be used by academic researchers. This came to be the start up of academic supercomputing within Sweden.

The Cray-1 was used until 1989. After removing classified components the Cray-1 central unit was displayed at the university and IT-ceum in Linköping until it was finally transferred to Tekniska museet in Stockholm in December last year. Visit the exhibition there, it's a nice one. And talk to our first "super".

KARL-FREDRIK BERGGREN

we have shown in a joint experimental and theoretical study that an 18 nm long conjugated polymer has still quantized electronic structure and it behaves like a ballistic quantum transport device[5]. Such a behavior is a result of strong delocalization of pi orbitals in polymer. The size of an 18 nm long conjugated polymer is not an easy task for theoretical modeling. To meet the challenge, we have developed a conceptually simple but very efficient computational approach (named as central insertion scheme (CIS) and implemented in BioNano-Lego program of our group) that allows to calculate quasi-periodic finite systems of very large size (up to 200.000 electrons) at density functional theory levels[6,7]. One of the applications is the evolution of electronic structure of single walled carbon nanotube (SWCNTs) with respect to its length, as shown in Figure 3. For the given tube, it is noted that discrete orbitals still occur even at the length of 10 nm. An oscillation of band gap is observed for this metallic tube and their molecular orbitals become even more delocalized for longer tubes. With CIS, we have calculated electronic structures of 77 types of SWCNTs with diameters less than 1.2nm at hybrid density functional theory level, which have helped to analyze and to interpret a set of experimental data. We are currently working on the design of functional molecular devices using CNTs as electrodes.

The main contributors in our group to the work presented here are Dr. Jun Jiang, Dr. Mathias Kula, Bin Gao, and Hui Cao. Generous support from national supercomputer facilities, NSC, PDC and HPC2N, is highly appreciated.

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Yi Luo is professor in theoretical chemistry at the school of Biotechnology, Royal Institute of Technology.

Neolith Status

It is now late February, and Neolith is inching into full production. The last few months have been filled with interesting challenges and some unanticipated problems.

Even before the start of the Neolith project it was clear that NSC needed more space and cooling capacity, and that a new server room was needed. Because of this, Neolith would be installed in two stages; stage one, to be installed in our old server room, and stage two to be installed when the new server room was finished.

This would also enable us to test the various system components under production conditions before the final installation. Since real production conditions for a large cluster are very complex and difficult to emulate with a synthetic load, we turned to our users for assistance. Providing test users with early access to the cluster would help us identify possible system bottlenecks or problems, and the users would get free CPU hours in exchange for providing us with frequent and detailed technical reports.

So, one day in early summer, stage one was delivered and installed next to Mozart. Initial hardware testing and a week long stress test didn't reveal very much out of the ordinary; a few bad CMOS batteries and a few dead memory modules.

Soon after the first shake down, the first test users were given access to the system and as summer passed and the new server room started to materialize, our cluster software began working much as expected.

In September, two and a half truckloads of hardware were unloaded and rolled into the building. Installation of Neolith stage two started. It took the better part of three weeks for vendor staff to label and connect all the cables in the cluster. It was pretty amazing that the 1600 cable InfiniBand fabric just worked when initially powered on!

A while after bringing it all on-line we however started to notice something unexpected. Some machines would occasionally log an uncorrectable memory error. Strangely, nothing of this was ever seen during the extensive memory testing that we had performed earlier, and the errors were also hard to reproduce. NSC staff and the vendor have spent a large amount of time tracking this problem down.

We are now close to having all the major hardware problems fixed, and are currently focusing on putting the last missing pieces of the software environment together. Much thanks to insightful user feedback, we will finally have the system in full production within the near future.

MATTIAS SLABANJA

UPCOMING EVENTS

SIAM Conference on Parallel Processing for Scientific Computing

March 12–14, 2008, Atlanta, Georgia, USA.
http://www.siam.org/meetings/pp08/

MOLCAS Workshop

April 14–18,2008, Lund, Sweden.
http://www.lunarc.lu.se/Courses/molcas-workshop

HPCS 2008; High Performance Computing and Simulation Symposium

April 14–16, 2008, Ottawa, Canada.
http://hosting.cs.vt.edu/hpc2008

HiCOMB 2008; 7th IEEE International Workshop on High Performance Computational Biology

April 14–18, 2008,Miami, Florida, USA.
http://www.hicomb.org

IPDPS 2008; 22nd IEEE International Parallel & Distributed Processing Symposium

April 14–18, 2008, Miami, Florida, USA.
http://www.ipdps.org

JSSPP 2008; 14th Workshop on Job Scheduling Strategies for Parallel Processing

April 18, 2008, Miami, Florida, USA.
http://www.cs.huji.ac.il/~feit/parsched/jsspp08/

ACM International Conference on Computing Frontiers

May 5–7, 2008, Ischia, Italy
http://www.computingfrontiers.org/

Workshop "Memory Access on future Processors: A solved problem" at ACM International Conference on Computing Frontiers

May 5–7, 2008,Ischia, Italy
http://www.lrr.in.tum.de/~weidendo/cf08/

I-SPAN 2008; The 9th International Symposium on Parallel Architectures, Algorithms and Networks

May 7–9, 2008, Sydney, Australia.
http://www.cs.usyd.edu.au/~ispan08/

CCGrid'08; 8th IEEE International Symposium on Cluster Computing and the Grid

May 19–22, 2008, Lyon, France.
http://ccgrid2008.ens-lyon.fr

ISC'08; International Supercomputing Conference

June 17–20, 2008, Dresden, Germany.
http://www.supercomp.de/isc08/index.php5

SC 08; International Conference for High Performance Computing, Networking, Storage and Analysis

November 15–21, 2008, Austin, Texas, USA.
http://sc08.supercomputing.org

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