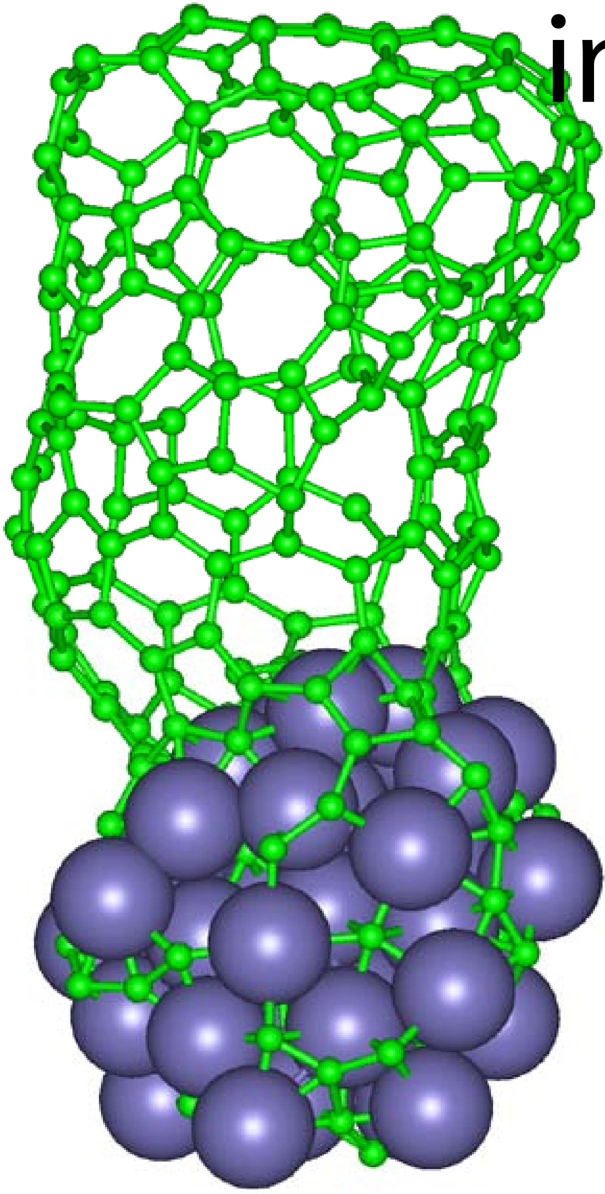
NSC News

National Supercomputer Centre at Linköpings universitet

2006:4

A Large Interest in Small Things



Nanoscience is not primarily concerned with decreasing the size of existing systems, but rather the identification, development and implementation of new materials with novel properties.

Kim Bolton has been using Monolith and Sgi3k at NSC, as well as Ra at Uppmax, to study novel properties, growth and manipulation of carbon nanotubes. These facilities have also been used to study ice-catalysed reactions relevant to stratospheric ozone depletion, phase equilibria and water penetration into polymer matrices (see www.adm.hb.se/~kib).

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LCSC'06

In October, NSC arranged the workshop Linux Clusters for Supercomputing, LCSC, for the seventh year running. Professor Thomas Sterling gave a keynote presentation in which he sketched the future use of multi-core technology in Beowulf clusters.

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Terabytes galore

Using a new parallel file system, Lustre, NSC now offers SMHI users access to high performance multi-TiB contiguous storage areas.

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The Future

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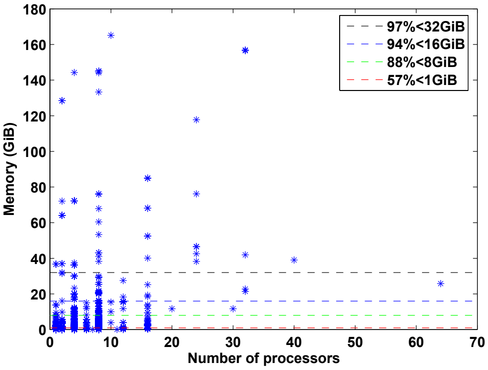
This is written on my way back from the Supercomputing Conference, SC'06 in Tampa, Florida. The Supercomputing Conference series is the most important annual meeting in the supercomputing community. Altogether 6 people from NSC went to SC'06. I think it is important that our staff has the possibility to, at least once, participate in "the event" in supercomputing, it gives the perspective that what we are doing is important both from a scientific perspective and commercially.

Apart from the technical trends presented at SC'06, summarized below by Niclas Andersson, there was definitely also a trend to present predictions about the future. In the keynote address Ray Kurzweil, one of the most successful and famous inventors in the US, showed how the paradigm shift rate has been doubling every decade and based on this observation he could predict that the twenty-first century will see 20,000 years of progress at today's rate! What kind of computer will we have in 2100? In another session, entitled HPC Computational Systems of 2020, experts such as Thomas Sterling (the father of Beowulf clusters and also the keynote speaker at our LCSC'06 workshop, see article below) predicted the design of the best HPC architectures in 2020. I came a bit late to this session and people were already queuing to enter the completely filled room. There is definitely a large interest in the future. Due to my late arrival I could not attend the session and I have to wait and see!

A near future perspective was taken in the session Multi-Core for HPC: Breakthrough or Breakdown? The main question was: Can multi-core span the next decade of Moore's Law progression? In the short-term NSC perspective I can make the following prediction about the effect of multi-core technology: Duolith, our new capability system that will be available from July, 2006 will beat the Moore's law progression of the Monolith capacity!

The main article in this issue of NSC News is written by Dr. Kim Bolton. In addition to the short presentations of SC'06 and LCSC'06 introduced above, Peter Kjellström presents one of the recent development projects that was completed at NSC, deployment of the Lustre parallel file system. We also take this opportunity to guide the users of Mozart in which kind of applications that are best suited for the SMP system. If everybody follow these guidelines, the availability of Mozart will be far better than today.

Even though I felt tempted to stay in sunny Florida over the darkest part of the Swedish winter, the Christmas items in the show-windows in Tampa seemed misplaced in the "summer" weather and I have no problems going back. A few weeks of intense work is waiting followed by a break for the holidays. I therefore take this opportunity to whish all of you; users, partners, and friends a Merry Christmas and a Happy New Year!



Efficient use of Mozart

After nine months in service it stands clear that Mozart is a very popular resource among SNAC users, and its popularity does in fact affect its availability. In order to maximize the scientific output, we, as a user community, should therefore make sure to restrict the use of Mozart to jobs that require large memory and direct other jobs elsewhere. The statistics reveal that 57% of the jobs on Mozart have used less than 1 GiB of memory (see figure), and, for the benefit of everyone, this category of jobs should without exception run on other resources.

Carbon nanotube growth mechanis

In 1985 Nobel laureates Curl, Kroto and Smalley discovered a new type of carbon material called fullerenes, and this was followed six years later by the discovery of a second type of carbon nanomaterial called carbon nanotubes (CNTs). These can be thought of as shells of seamlessly rolled up layers of graphene, as illustrated in Fig.1. The CNTs that were produced in the pioneering experiments by Iijima in 1991 consisted of many concentric graphene walls and are therefore called multi-walled CNTs (MWNTs). In 1993 single walled CNTs (SWNTs) were produced by both the Iijima and Bethune groups.

Different chiralities

Fig. 1 shows three types of SWNTs, classified by their (n,m) chiral indices (these indices will not be discussed here, but all SWNT structures – called *chiralities* – can be uniquely identified by their chiral indices). In panel a, the graphene sheet is folded around its vertical axis to form a (10,0) SWNT. Due to the shape of the SWNT ends, it is called a zig-zag type nanotube. Rotation of the graphene sheet by 90° and folding around the vertical axis leads to the (5,5) arm-chair type SWNT shown in panel b. Panel c illustrates the formation of the (7,3) SWNT.

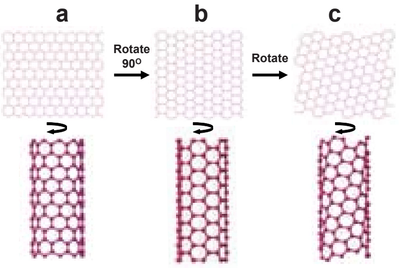


Figure 1. Illustrating the formation of SWNTs from graphene sheets.

Similarly to the carbon fullerenes, SWNTs are not merely a miniaturisation of graphite or diamond, but are new materials with unique properties and potential technological applications. This is due, for example, to the quantisation of electronic states around the nanotube circumference, the fact that all atoms are on the surface of the tube and, neglecting defects, the SWNT forms a perfect sp^2 carbon bonded system. Depending on their chirality, SWNTs are either large gap semiconductors or metallic, making them potential components in electronic circuitry. The electronic properties can be identified by the chiral indices shown in Fig. 1: an (n,m) SWNT is metallic if n–m is a multiple of three, otherwise it is semi-conducting.

It is this property, together with their good thermal conductivity, that has aroused the most interest in SWNTs and also posed the most challenges. One of the major hurdles to using SWNTs in electronic devices is that all known production methods yield a mixture of nanotube structures. There is also no efficient method to separate SWNTs based on their chirality. A holy grail is to grow SWNTs, with desired chiralities, at the required positions in the electronic circuit. This is a major challenge since SWNTs are grown from catalytic metal nanoparticles at high temperatures, and atomic-level changes during the growth process can alter the chirality and, hence, the electronic property of the SWNT.

Computational methods complement experiments since they offer easy manipulation and analysis at the atomic level. We have used the NSC facilities to study SWNT properties relevant to sensor devices, as well as their chiral-dependent manipulation and growth. Although we have used a variety of computational methods, the present discussion focuses on our molecular dynamics (MD) calculations of SWNT growth.

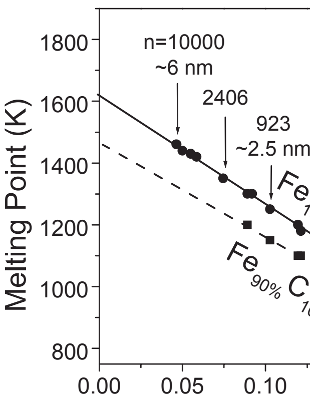
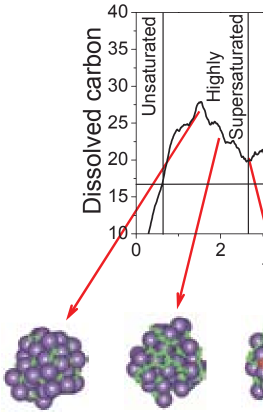


Figure 2. Linear decrease in iron
inverse cluster diameter (the dia
number of cluster atoms).

Figure 3. Snap shots of SWNT nuc
900 K. The inset shows the numb



The Lustre File System in production at NSC

Lustre is a very scalable parallel file system developed and supported by Cluster File Systems Inc. (CFS). Lustre is available under the GPL and as a commercial product from CFS (HP also sells it under the SFS name). Lustre is designed for performance and scalability and is used on many of the most powerful machines on the top500 list. The current limits/records are approximately 100,000 clients, 4,000 I/O-servers, 100 GB/s and more than 1 PB in one file system. A Lustre file system consists of one meta-data server (with optional fallback), one or more object storage servers (where all the data is stored) and one or more clients. When a file is stored on a Lustre file system it can either be as one object (on one object server) or split up into many objects (and striped over as many object servers). How this is handled can be configured on a per-file basis and controlled by the user. Striped files are generally more expensive to manage (meta-data-wise) but can be accessed with greater bandwidth.

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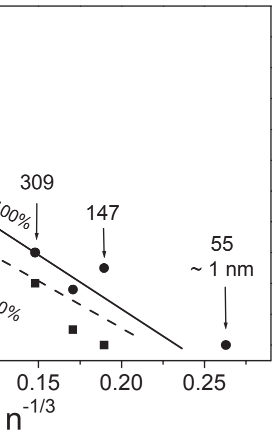
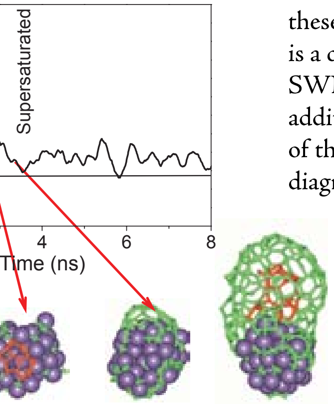


and iron-carbide melting points with the
meter is proportional to the cube of the

cleation and growth from an Fe_{50} cluster at
er of dissolved carbon atoms over time.



As mentioned earlier, SWNTs are grown from metal nanoparticles. These particles act as catalysts for the decomposition of carbon feedstock, solvents for the decomposed carbon species and as templates for carbon nanotube growth. It is essential that the force field used in the MD simulations correctly describes the trends in the melting behaviour and metal-carbide phase diagram (both of which can strongly influence the SWNT growth mechanism). As shown in Fig. 2, the potential model yielded the correct linear decrease in cluster melting point with the inverse cluster diameter (Fe was used in these studies since this is a common catalyst in SWNT production). In addition, the correct form of the iron-carbide phase diagram was obtained, with a eutectic point at ≈12% carbon concentration. This leads to the lower cluster melting points for 10% carbon concentration shown in Fig. 2.

Fig. 2 shows that small particles (55 atoms ≈ 1 nm) melt at temperatures below 800 K and larger particles (2500 atoms ≈ 6 nm) melt at temperatures above 1400 K. Since common SWNT production methods use temperatures and particles in this range, the simulations reveal that both liquid and solid catalyst particles may play a role in the growth mechanism.

Fig. 3 shows typical snap shots of SWNT nucleation and growth from an Fe_{50} particle at 900 K, which is above the cluster melting point. As seen in the inset, the first 15 C "feedstock" atoms dissolve in the cluster. When the iron-carbide (Fe-C) cluster becomes supersaturated in carbon, C atoms precipitate to the surface, but are not stable and redissolve into the cluster. Only when the cluster is highly supersaturated are there a sufficient number of precipitated carbon atoms for them to interact and form bonds (see the structure at about 1.5 ns). These carbon strings are stable on the surface and act as nucleation sites for further precipitation and growth of longer strings, carbon polygons and eventually a SWNT cap that elongates into the nanotube.

> *…new materials with unique properties and potential technological applications*

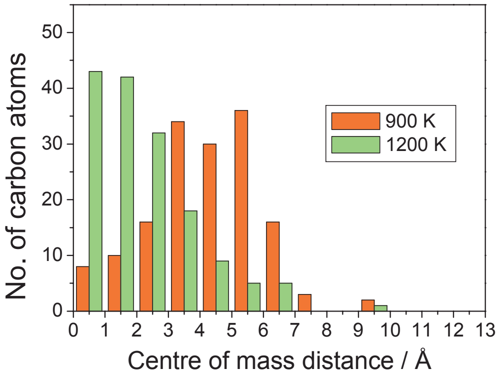


Figure 4. Histogram of the minimum separation between the cluster centre of mass and the carbon atoms before they join into the SWNT. Results are for solid and liquid Fe_{300} clusters at 900 and 1200 K, respectively.

Growth from solid iron

A similar mechanism is observed for SWNT growth from solid Fe particles, since metal nanoparticles have liquid-like layers below their melting points. The only major difference is that, for the solid particle, carbon atoms do not diffuse into the centre (bulk) of the metal cluster before becoming part of the growing SWNT structure, but diffuse to the SWNT end along the cluster surface. Fig. 4 is a histogram of the minimum centre of mass separation that the carbon atoms have before

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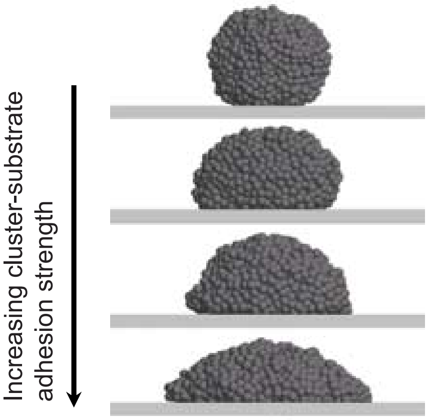
Lustre is now available on two clusters at NSC, Tornado (Climate modelling) and Dunder (SMHI research and development). The configuration consists of eight object storage servers and two meta-data servers. The total (raw) storage capacity is 56 TB (TB = 1000^4 B) and this is split up into four different file systems totaling 35.8 TiB (TiB = 1024^4 B) of user available space.

Both software and hardware have worked well for us but a lot of time has been spent configuring and tuning the file system. Managing and upgrading the clusters has also become more complex and we eagerly await the next major Lustre release which will support so called "patch-less" clients (today Lustre requires clients to run a modified OS kernel). From a user perspective it seems the two most obvious differences (compared to our current generation of NFS servers) are the size (one Lustre file system instead of several NFS file systems) and the fact that Lustre remains interactive during high I/O load. Overall the implementation of Lustre at NSC has been a success and we will definitely consider it for coming storage systems.

PETER KJELLSTRÖM

Figure 5. Adhesion to a substrate leads to flattening of the cluster.



joining into the SWNT. It is for an Fe_{300} cluster (melting point 1100 K) and shows that most carbon atoms remain near the cluster surface when the cluster is solid and diffuse into the bulk when the cluster is liquid.

The above simulations are of SWNT growth from an isolated (free) metal particle. However, most production methods use supported catalytic particles, and we are therefore studying the effect of the substrate on the growth mechanism. Our results indicate that the major effect of a flat, neutral support is to flatten the metal cluster and increase its melting point. The change in shape of a liquid Fe_{2000} cluster with increasing substrate-cluster adhesion strength is shown in Fig. 5. The growth mechanism from supported iron clusters is thus very similar to that from isolated clusters, but an isolated cluster that is liquid may become solid when supported on a substrate.

Future work and acknowledgements

Work on SWNT growth mechanisms is continuing in our group. In particular, we are focusing on simulating the growth of SWNTs with determinable chirality, which requires combined DFT, MD and Monte Carlo approaches .

The work described here was done primarily by Dr. Feng Ding, who is now at Rice University in Texas, USA. Other recent and current contributors from our group are Arne Rosén, Simon Gustavsson, Haiming Duan, Wuming Zhu and Anders Börjesson. National and international collaborators include Eleanor Campbell (Göteborg University), Peter Eklund (Pennsylvania State University), Christophe Bicharre (CNRS, France), Stefano Curtarolo and his group at Duke University, and Avetik Harutyunyan and Toshio Tokune from Honda Research Inc.

We are grateful for funding for this project, which comes from the Swedish Research Council, the Swedish Foundation for Strategic Research, Honda Research Institute USA Inc. and the Particles in Interactive Environments platform at Gothenburg University. This work could not have been done without the resources allocated at the Swedish National Supercomputing Facilities, including the NSC supercomputers.

Kim Bolton is professor in Physical Chemistry at the School of Engineering, University College of Borås. He is also guest professor in the Department of Physics, Göteborg University.

A Visit to Supercomputing 2006

Supercomputing 2006 is the premier international conference on high performance computing, networking, storage and analysis. This year's conference is the second largest since the meeting was first held in 1988, with more than 7,100 badged attendees filling the Convention Center in Tampa, Florida. The conference program consists of a multitude of threads; technical papers, masterworks, invited speakers, panels, workshops, awards, birds-of-feathers, educational program, posters, and more. But the most impressive of the event is the show-floor. 274 exhibitors covers the 18.500 square meter exhibit hall. Each year SCinet builds the world's most advanced technology network on-site. Vendors and research labs from around the globe with products and projects pertaining to supercomputing gathers together during the three days the exhibition is open.

The hottest topic in discussions at SC06 is that all common processors now include multi-core technology in their road-maps. Clock frequency is no longer the the principal path for increased performance. Instead, 2-8 cores per chip is available today. But that is merely a start. There will be hundreds of cores on each silicon chip within five to six years. This will put a lot of strain on programmers and programming environments. How do you efficiently use a computer cluster with hundreds of thousands of cores?

Another hot topic is the use of specialized hardware for computing. Not only by fitting kernels into FPGAs but also using programmable graphic processors for high performance computations. A very attractive architecture is IBM's new Cell processor which was initially designed for Sony's Playstation 3, currently released in Japan and USA. The Cell processor will most likely appear in many more advanced consumer appliances as well as a vehicles for performance in high performance computer systems.

Conference website:
http://sc06.supercomputing.org

NICLAS ANDERSSON

UPCOMING EVENTS

IPDPS 2007; 21st IEEE International Parallel & Distributed Processing Symposium

March 26–30, 2007. Long Beach, California, USA.
http://www.ipdps.org/

CAC 2007; The Workshop on Communication Architecture for Clusters

March 26–30, 2007. Long Beach, California, USA.
http://www.c3.lanl.gov/cac2007/

HCW 2007: The 16th International Heterogeneity in Computing Workshop

March 26, 2007. Long Beach, California, USA.
http://navet.ics.hawaii.edu/hcw2007/

HiCOMB 2007; 6th International Workshop on High Performance Computational Biology

March 26, 2007. Long Beach, California, USA.
http://www.hicomb.org/

ACM International Conference on Computing Frontiers

May 7–9, 2007, Ischia, Italy.
http://www.computingfrontiers.org/

CCGrid07; 7th IEEE International Symposium on Cluster Computing and the Grid

May 14–17, 2007, Rio de Janeiro, Brasil.
http://ccgrid07.lncc.br/

Workshop on Linux Clusters for Super Computing

For the seventh consecutive year, NSC arranged the workshop Linux Clusters for Supercomputing, LCSC. On October 18 we had two tutorials, Optimization of shared memory systems and Gaussian 03, presented by Alexis Cousein and Roberto Gomperts, respectively. Both of these events were presented by SGI with the intention that Mozart users should get a more detailed understanding of the usage of an SMP system.

The workshop on October 19 was focused on technical aspects of supercomputing. We had the great pleasure to have professor Thomas Sterling from Louisiana State University as the keynote speaker. Thomas gave a stimulating presentation entitled Multi-core Beowulf Clusters for Petaflops-scale Computing. Another international guest, Juan Jose Porta from IBM and Barcelona Supercomputing Center, presented the new IBM Cell processor. The title of his presentation, From Gaming to Serious Supercomputing Fun, indicates the width of the application of the Cell processor.

One session was devoted to recent Nordic HPC initiatives. Cyril Banino-Rokkones presented the new Norwegian HPC system at NTNU in Trondheim, Juha Fagerholm presented the recently finalized procurement at CSC in Finland, Lars Fischer gave an overview of the activities at the Nordic Data Grid Facility, NDGF, hosted by NORDUnet A/S in Copenhagen. Finally, Sverker Holmgren, the SNIC director, presented the Swedish HPC landscape and roadmap.

From the organizers' point of view we are very satisfied with the event. The focus on technical aspects of HPC was to some extent motivated by the fact that SNIC Interaction, the annual users-group meeting, was arranged shortly after our workshop. However, we got the impression that many of the participants liked this narrower scope and in view of the focus of SNIC Interaction we might keep this format even next year. There will be a LCSC'07, which also will involve inauguration of our next HPC resource, Duolith.

Finally, we would also like to take this opportunity to thank our sponsors IBM, SGI and Dell and all the speakers for their contributions.

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