NSC News
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Peak Performance

NSCs new supercomputing cluster, Neolith, has ranked higher on the Top500 list than any Swedish academic system ever has.

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Atomistic Spin Dynamics

Olle Eriksson is studying magnetization properties of solid materials in new ways.

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Moving On

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About a month ago NSC arranged the LCSC workshop and performed the inauguration of our new capability resource, Neolith. We had a great meeting with interesting presentations and lively discussions. The "switch on" of Neolith by Pär Omling, Director General of the Swedish Research Council and Mille Millnert, Rector of Linköping University was of course the highlight of the meeting and also an important milestone for NSC. During the workshop we speculated about how high on the Top-500 list we could get this time, previously our top positions have been 35, with the Cray T3E in 1997 and 51 with Monolith in 2002. Even though the guesses were somewhat spread all agreed that Neolith would give us a new all time high position, and it did, we ended up as number 23 on the list of the fastest computers in the world. This has given us a lot of attention, and I must say that it is a nice feeling to be among the strongest centres in the world of HPC – all credit to the skilful and hard working staff at NSC for this amazing achievement.

I have now decided to move on in my career and I will leave NSC after 4 years. It has been a fantastic time here, I have learned a lot, met a lot of great people, and hopefully also contributed to the development of NSC during my time here. I would like to take this opportunity to thank all my colleagues, the NSC board, all the SNIC people, all our academic users as well as the users and collaborators at SMHI and Saab. It has been a wonderful time that I, whenever I come in the mood of looking back at things, will remember with great pleasure.

Neolith inauguration and LCSC'07

Neolith, the new main NSC resource was inaugurated on October 17 by the director of the Swedish Research Council, Pär Omling. He pointed out the great value of access to state of the art HPC resources for Swedish researchers. Mille Millnert, rektor of Linköpings universitet, added local perspective. The manufacturer Hewlett-Packard were represented by Peter Noring and Jan Wallenberg while the technical director of NSC, Niclas Andersson, gave a technical presentation of the system. The inauguration ended with an indoor firework and the display of a performance meter ramping up to the 60 TFlop/s peak performance of Neolith.

The inauguration took place as a part of the 8:th annual 'Linux clusters for supercomputing' workshop, LCSC, 16-18 October. The program contained tutorials, the inauguration, presentations of international outlooks on HPC and on technical aspects of HPC, as well as more user and application oriented presentations.

We would like to take this opportunity to thank our sponsors HP, IBM, Intel, GoVirtual and Nexsan and all our speakers for their contributions to LCSC.

PETER MÜNGER

New staff member: Jens Larsson

I have been working part time at the National Supercomputer Centre since the beginning of November. For the past ten years I have been a system administrator at the Department of Electrical Engineering at Linköping University.

My first task will be a refurbish of the internal computer resources and the network infrastructure at NSC and then I will be involved with the Swegrid 2 upgrade.

Atomistic Spin Dynamics

Experimental Background

With the increasing interest in advanced magnetic materials for data storage and processing, there is an increasing need for a detailed microscopic description of magnetic materials. One of the more challenging aspects concerns magnetization switching and magnetization dynamics, where both experimental and theoretical aspects pose a difficulty. Magnetic switching is the process of moving a system from one stable magnetic configuration to another and is fundamental for any system where a magnetic state is used for storing and retrieving information. The switching process involves an excitation of the system followed by a relaxation into a new stable configuration. Often the switching is induced by a pulsed external magnetic field. After a short magnetic pulse, the spin-system relaxes into a new stable configuration. Recent experiments have demonstrated the ability to switch magnetic configurations at tremendous speeds, of the order of tens of femtoseconds.[1]

The commonly used approach for studying magnetization switching and spin dynamics is called micromagnetism, and it provides a framework for understanding magnetization dynamics on length scales of micrometers. The approach, however, suffers from a number of limitations, and it would be desirable with a microscopic approach based on the quantum description of solids, an approach which properly displays the connection between the electronic structure of the material and the magnetization dynamics. The scope of this short text is to give a brief presentation of a methodological and computational scheme for performing spin dynamic simulations on an atomistic scale.[2] The approach is based on an atomic scale description of the magnetization of a solid.

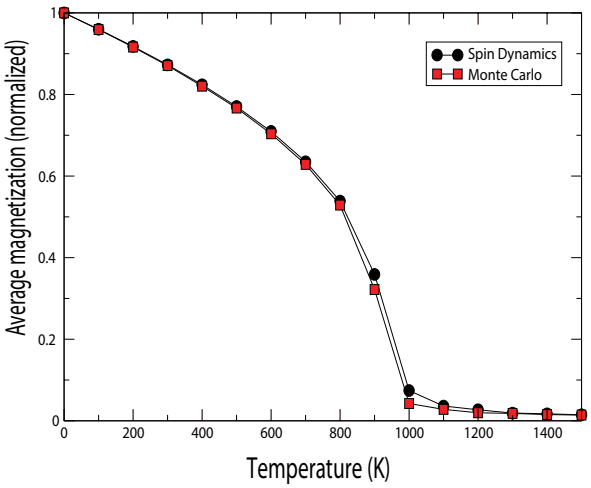

Figure 1: Comparison of equilibrium magnetization versus temperature for a periodic 20×20×20 bcc Fe system for SD and MC.

Atomistic Spin Dynamics

The starting point of deriving the spin dynamics equations is the commutator between the spin operator and the Hamiltonian of the system. After some algebra one can from this starting point derive the equation of motion for the orientations of the atomic moments, $\mathbf{m}_i$,

$$\frac{d\mathbf{m}_i}{dt}(t) = -\gamma \mathbf{m}_i(t) \times \mathbf{B}_i,$$

(equation 1)

where i denotes atomic index, γ is a proportionality constant called the gyromagnetic ratio, and $\mathbf{B}_i$ the effective field which the moment $\mathbf{m}_i$ experiences.

This field is primarily due to exchange interactions with other atomic moments in the lattice, and is calculated from

$$\mathbf{B}_i = \frac{\partial \mathscr{H}}{\partial m_i}.$$

(equation 2)

The Hamiltonian contains interactions describing interatomic exchange, magnetic anisotropy, dipolar interactions and the coupling between atomic moments and an external field. In order to make the approach truly first principles one should preferably calculate all these interaction terms, something density functional theory enables one to do.[3]

Finally we note that dissipation of energy from the system can be modeled by adding a phenomenological Gilbert damping term to Eq. 1, resulting in,

The new SNAC application system

The new application policy for HPC resources was used for the first time this autumn. The Swedish National Allocation Committee for HPC, SNAC, now considers three categories of applications – large scale projects, medium scale projects and small scale projects.

Calls for large scale projects are issued twice a year, in April and October, resulting in allocations effective from January 1 and July 1 respectively. Large scale applications are evaluated by two scientific referees from the SNAC committee and one technical referee from a Swedish National Infrastructure for Computing, SNIC, member center. Currently the lower limit for large scale applications is 40.000 core hours/month for all resources apart from the very special Mozart at NSC with a limit of 5.000 core hours/month. As a rough guide, half of the resources are devoted to large scale projects. In the very first call for large scale applications this autumn 17 out of 20 applicants applied for time on NSC resources! The ratio

$$\frac{d\mathbf{m}_i}{dt} = -\gamma[\mathbf{m}_i \times \mathbf{B}_i] + \frac{\alpha}{m}[\mathbf{m}_i \times \frac{d\mathbf{m}_i}{dt}],$$

(equation 3)

where α is the damping coefficient. Although attempts have been made to calculate also the damping term, it is fair to say that this is a very demanding task in general, and in the examples provided here we have used α as a parameter. All other terms in the Hamiltonian are calculated from density functional theory.

Computational aspects

Simulations of atomistic spin dynamics are inherently heavy computations. To incorporate finite temperature and dissipation effects, the equations of motion, Eq. 3, are coupled to a heat bath, transforming the equations to a set of coupled stochastic differential equations. In simulations made so far, the number of magnetic moments was of the order of ten thousands and the number of time steps counted in millions. The obvious way to parallelize this algorithm is to decompose the set of magnetic moments over the processor cores. The present implementation is an advanced prototype where the ambition is to have a full-fledged MPI-version ready in the first half of 2008. The long execution times for the present serial program has so far been tackled by parameter variation and scripting. The program flow scheme is very much reminiscent to standard Monte Carlo methods for lattice systems. The main challenges are found in optimizing the single processor core performance and obtaining memory parallelization for those subroutines where it is necessary.

Results

As an example of how spin-dynamics simulations perform, we show in Fig. 1 the saturation magnetization for bcc Fe versus temperature. The simulations were performed on a bcc crystal where the conventional unit cell has been doubled twenty-fold, in the x-, y- and z-directions. In Fig.1 we also plot the magnetization curve for a Monte Carlo simulation (with the same exchange field as in the spin-dynamics simulations). It may be seen that the two simulation methods result in identical magnetization curves. Fig. 1 also shows that the ordering temperature, i.e. the temperature where the magnetism disappears, of bcc Fe lies close to 1000 K in the simulations, which is in rather good agreement with the experimental value of 1043 K.

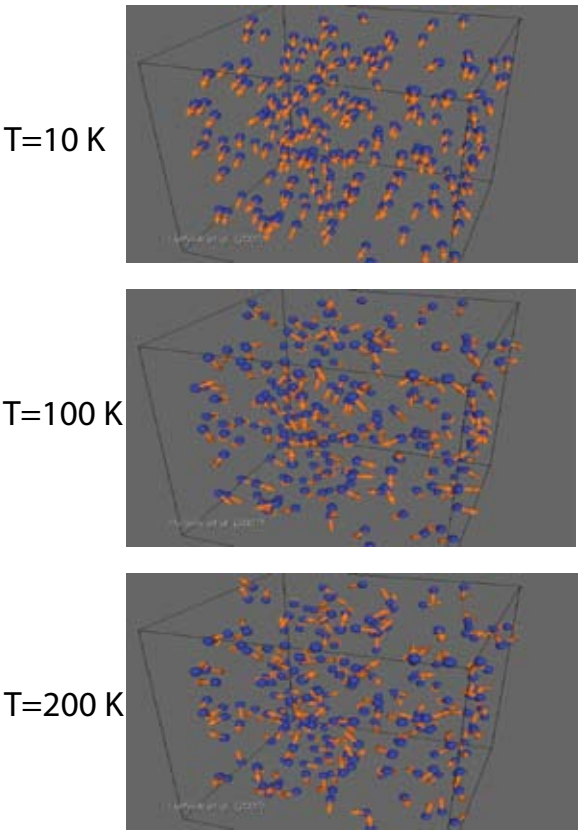

Figure 2: Snap shots of spin configurations of a spin dynamics simulation of Mn (5%) doped GaAs. In the top pane the simulation was done for T=10 K, in the middle panel T= 100 K was used, and in the lower panel the temperature was 200 K. The ordering temperature for the system was calculated to ~ 150 K.

Another example of spin-dynamics simulations is shown in Fig. 2, where snap-shots of spin-configurations of Mn doped GaAs, a diluted magnetic

between time applied for and time available was 2.9 on Neolith and 6.8 on Mozart.

Applications for medium scale projects can be submitted at any time directly to the center with the requested resource. The evaluation will be carried out by application experts at the centers and assess the feasibility of using the requested resources for the proposed purpose. The upper limit for medium scale projects is currently 5.000 core hours/month on Mozart and 40.000 core hours/month on all other SNIC resources. Work is in progress at the SNIC member centers on an unified electronic application systems for medium scale projects.

Small scale projects, i.e. less than 2000 core hours/month, on all systems apart from Mozart where the limit is 250 core hours/month, are handled by the SNIC member centers. Applications can be submitted directly to the centers at any time during the year.

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semiconductor, are shown. Note that spin configurations are shown for three different temperatures. In this figure only the magnetic Mn atoms are shown, Ga and As atoms are invisible. At low temperature a ferromagnetic state has the lowest total energy, which in Fig. 2 is signaled by the fact that most atomic spins are parallel to one another. The disorder among the different spins is increasing with temperature and at T=100 K most spins point in random orientation whereas at T=200 K the spin arrangement is completely random. The ordering temperature in these simulations is ~150 K, which is in decent agreement with the observed value of 170 K. A real time animation of the simulations shown in Fig.2 can be downloaded from www.fysik.uu.se/theomag/asd.

The examples of atomistic spin-dynamics simulations presented here have focused on materials specific investigations of magnetization dynamics as a function of temperature. Hence the correlation between different spins in the simulation cell can be extracted as a function of time and distance, usually in a property referred to as a dynamic spin-correlation function. The application where atomistic spin-dynamics simulations is expected to have the largest impact, however, is for studies involving ultra fast magnetization switching, where a direct connection to experimental observations may be made, and possibly novel routs and materials for ever faster switching dynamics can be identified.

Acknowledgements

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Olle Eriksson received his PhD at Uppsala University 1989. He is currently head of the Theoretical Magnetism group at The Physics Department of Uppsala University. His research interests lies in electronic structure theory of materials, and related properties like magnetism and chemical binding.

Supercomputing 2007 and the Top500 list

Reno, "The Biggest Little City in the World" was this year's venue for the Supercomputing 2007 conference, with a record attendance both in terms of attendees (approx. 9000) as well as exhibitors (318).

There was no mistake that there was a very positive and upbeat tone to this year's conference, probably much due to the fact that the world economy is still going very strong. As usual the technical programme had a very comprehensive agenda with keynote, invited talks, technical papers, vendor presentations, BOF (Birds of a Feather) sessions, posters, tutorials and of course the exhibition.

The Supercomputing conference in general seems to be attracting a broader attendance for each year. This year was no different where presentations and exhibitions covered a broad set of products, ideas and visions. Linux clusters are abundant but MPP:s from vendors like the Cray XT5, IBM BlueGene and newcomer SciCortex are still attracting quite an interest. Vector systems also maintains a presence in the market. One frequent theme this year was clearly the availability and use of computing accelerators in various forms. Both FPGAs, GPUs, coprocessors and Cell-based architectures were presented and many of them now come with well established user environments and either existing or soon to be available 64-bit floating point capabilities. You still need a suitable application to be able to get access to very high performance using accelerators though. If you as a reader of NSC News think that your application could benefit from using an accelerator, please let us know so we can find out if we could do something fun together! Ideally the application should be compute bound and highly scalable such as image or signal processing applications.

One of the exciting events at Supercomputing is the release of the Top500 list and this year it was showtime for NSCs new Neolith system. Neolith performance of 44.5 Tflops (75 percent of peak) was achieved just prior to SC2007. At the press conference it was announced that Neolith achieved 23rd place which is the highest position ever achieved on Top500 by a Swedish supercomputer for academic use! Number 1 was the BlueGene/L from IBM at Lawrence Livermore which achieved 478.2 Tflops.

SC2008 will be in Austin, Texas. Wonder how many T-shirts I will get then?

Torgny Faxén

UPCOMING EVENTS

HiPC 2007; 14th IEEE International Conference on High Performance Computing

December 18–21 2007, Goa, India.
http://www.hipc.org

SIAM Conference on Parallel Processing for Scientific Computing

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

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/

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

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