NSC News

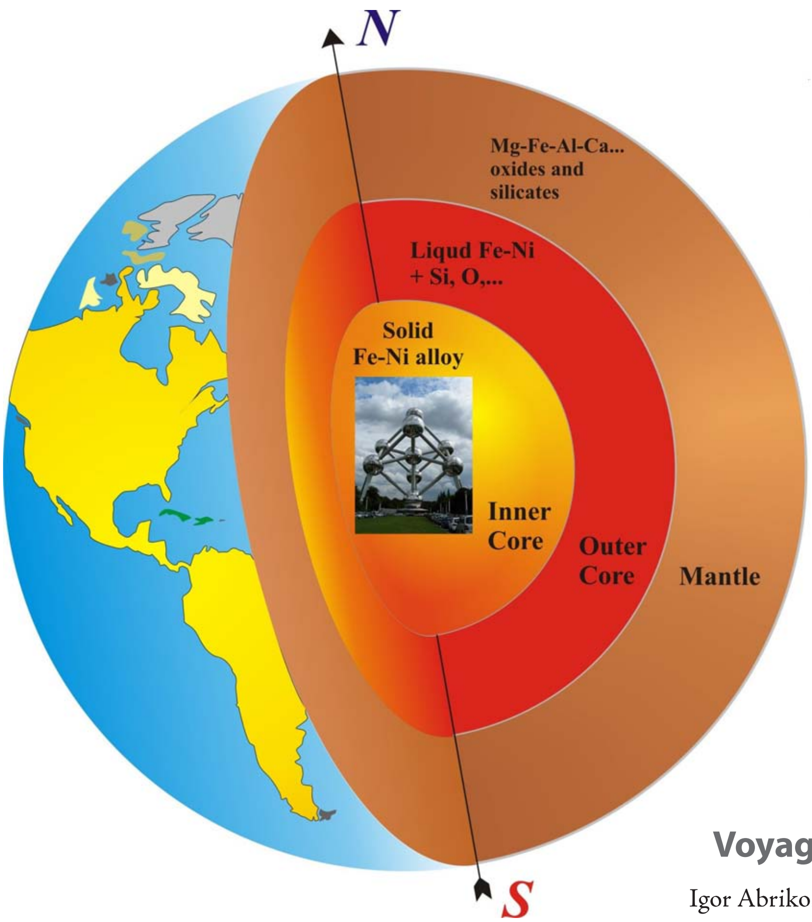
National Supercomputer Centre at Linköpings universitet

2008:3

NSC 08
SUNET
SUSEC

NSC'08 • SUNET TREFpunkt 19 • SUSEC Höstmöte • Linköping October 14–16, 2008

For more information and to register for the event, please visit http://www.nsc.liu.se/nsc08



Deep Down

Voyage to the Earth's Deep Interior

Igor Abrikosov is using NSC systems to study pure Fe and Fe-Ni alloys at extreme conditions inside the Earth's core.

Read further on page 3

New resources and projects to NSC

We are happy to announce that SNIC recently decided to finance a new high-performance computing resource at NSC. Of this new "foundation level system", half will be dedicated to local users at Linköping University and half to users country-wide achieving allocations via SNAC. The system will be used for bioinformatics, molecular dynamics, quantum chemistry, material physics, fluid mechanics and further disciplines, where it will match the growing demand from these users. With this welcome addition at NSC, we now have resources at all levels, making it smooth for users to move projects between different systems depending on the computational requirements. Thus, the resources can be utilised in a much more cost-effective manner.

Another happy announcement is that NSC has been granted to participate in the EU project IS-ENES aiming at creating an infrastructure for climate and Earth system modelling. This 20-partner project runs from 2009 to 2012 and will include development of distributed solutions for calculations and storage, where NSC will utilise its expertise in these areas. Furthermore, SMHI is partner in this EU project, making it an important extension of the collaboration between NSC and SMHI.

Now in September, the CERN experiments with the Large Hadron Collider (LHC) will start to generate exciting data. The data collection involves supercomputer centres all over the world, and NSC is one of these taking care of data acquirement and safe storage for subsequent analyses by participating research groups in Sweden and other countries. The data collection set-up in the Nordic countries is coordinated via NDGF (Nordic Data Grid Facility) and has been shown very successful and reliable in various tests performed before the real experiments that now start.

Finally, I would like to wish you very welcome to attend the NSC'08 workshop on large-scale storage solutions and the accompanying SUSEC autumn meeting and SUNET conference –three conferences during three days, 14–16 October at Linköping University.

BENGT PERSSON, DIRECTOR OF NSC

Breaking the Petaflop/s Barrier

In May this year, the IBM-built system Roadrunner at Los Alamos National Laboratory became the first supercomputer to achieve more than one petaflop/s sustained on the Linpack benchmark. This event resulted in the gold position in the June edition of the top500-list (www.top500.org) of world fastest supercomputers. It left the competition far behind: The second position on the list is held by a large IBM BlueGene/L system at Lawrence Livermoore National Laboratory achieving "merely" 478 teraflop/s on Linpack.

NSC's largest system, Neolith, hold the 40:e position on top500 with the sustained Linpack performance of 44.46 teraflop/s. In June it was surpassed by HPC2N's latest cluster, Akka, at position 39 with 46.04 teraflop/s. The fastest supercomputer in Sweden according to Linpack is still FRA's impressive cluster which is ranked no 11 on the list of world's fastest supercomputers.

New to the June edition of this list is that it has started to track measured power consumption values. Not too surprising, the fastest supercomputer on the list is also the most power-efficient system. Solving power distribution and heat dissipation is the most difficult challenge in the development of increasingly dense computing resources.

Next edition of top500 is published at the Supercomputer conference in November this year.

NICLAS ANDERSSON

New staff member: Johan Raber

I am joining NSC this September as a systems expert on distributed computing. My main responsibilities will be projects focussing on distributed data storage and backup solutions, but I will also work with the administration of the other computing resources at NSC. I come most recently from the Dept. of Cell & Molecular Biology at Uppsala University where I finished my PhD studies in biophysics, studies which heavily relied on distributed computing – computational chemistry, mainly – and this is also how I got in to this line of work .

Voyage to the Earth's Deep Interior

Early in the 20th century it became evident from the study of seismic waves that the interior of the Earth, similar to other terrestrial planets, has a chemically divided radially layered structure, like that of an onion (Fig. 1). The rock units and layers near the surface are understood from direct observations, core samples, and drilling projects. However the deepest drill hole has only reached less than 12 km below the Earth's surface. Thus, investigations of the conditions of the Earth's interiors (temperature, pressure, composition, density, rheology etc.) can be performed only through indirect means via studies of seismic waves produced by earthquakes, analyses of rocks, remains of meteorites etc. Besides laboratory experiments, theoretical simulations of physical properties of materials at extreme conditions are highly useful sources of knowledge about our planet.

The core is the most remote region on the Earth. A solid inner and liquid outer cores have radii of about 1220 km and 3400 km, respectively. Available cosmochemical, geochemical, and geophysics studies provide evidences that the Earth's core contains iron with substantial amount of nickel (5-20 %). Nowadays the extraordinary interest to the Earth's core is connected to advances in experimental high-pressure methods as well as to new developments in computer technologies and methods for theoretical modeling. It is currently possible to extend investigations leading to a new level of understanding of phase diagrams and structures of materials at extreme pressure-temperature conditions. This turns out to play extremely important role in studies of the processes like sound waves propagation and earthquakes, Earth's magnetic field behavior and magnetic poles swaps, and a so called nutation, or wobbling, of the Earth's rotation axis. A key issue in the understanding of these complex phenomena is the study of physical and chemical properties of different phases, which compose the Earth.

At the very high pressure and temperature conditions of the Earth's deep interior the accurate measurements of physical and chemical material properties become exceedingly difficult. Two widely-used techniques capable of generating such extreme conditions, shock compression and laser heating in diamond anvil cells, give certain discrepancies in results. On the other hand the main difficulty of theoretical simulations comes from extremely high temperature, which requires simultaneous consideration of the electron and ion motion. In principle, ab-initio molecular dynamics (AIMD) could treat all electronic and vibrational thermal contributions. However AIMD simulations require large number of atoms, long simulation runs, short time steps, as well as very high accuracy. All these requirements make the AIMD method about 4 orders of magnitude more time consuming than static methods, and therefore, such projects can be executed exclusively at high-performance computer facilities. Apart from this the study of the Eearth's core requires a proper treatment of disorder effects in alloys, which is still a challenging task.

In our Theoretical Physics group at IFM, Linköping University, we have been developing the theory of alloys and the unique methodology, which can be combined with AIMD simulations. In addition new powerful computer clusters, which are now available in Sweden and, particularly, at Linköping National Supercomputer Center (NSC) make it possible to perform realistic simulations in reasonable time. In our SNIC-supported project we have been performing ab-initio static and molecular dynamics calculations of the pressure-temperature phase diagram of pure Fe and Fe-Ni alloys at extreme conditions. Our very recent studies of these materials [1-2] shed new light on the structure of the Earth's core.

In particular, the text-book understanding of the Earth's solid core was that it should be composed mainly of the so-called hexagonal closed packed (hcp) Fe, i.e. Fe with the crys-

New staff member: Eva-Britt Berglund

Hi, my name is Eva-Britt Berglund and I am a new member of NSC. I will be working part time (50%) as an economist and the other 50 percent I will continue working at the Department of Computer and Information Science, IDA, at Linköpings universitet. I have been working at IDA during the last 17 years and today I work as an economist but also with public purchasing. I am looking forward to work with all of you!

tal structure of close-packed layers of atoms surrounded by hexagons of neighboring atoms. In collaboration with the experimental geophysics unit of Prof. L. Dubrovinsky and Prof. N. Dubrovinskaia from Germany we have performed a combined theoretical and experimental study of pure iron at different pressure-temperature conditions. We examined the face-centered cubic (fcc) crystal structure, another phase of Fe where atoms are arranged in cubes with all corners and all faces of each cube occupied by the atoms. The fcc Fe phase is known to be stable at ambient pressure and elevated temperature. We surprisingly revealed an extended region of stability of the fcc phase at pressure higher than 100 GPa [2]. Moreover a subtle energetic difference between different crystal structures of Fe may lead to a co-existence of several phases in the inner core (P = 300-360 GPa and T = 5000-7000 K).

Further an inclusion of Ni leads to stabilization of the body-centered cubic (bcc, see Fig. 1) structure of the alloy, as was demonstrated in Ref. [1]. Moreover, different light-element impurities, like Si [3], Mg [4], O, S, etc, are considered as possible elements, which can be present in the Earth's interior and which can strikingly influence the structural stability and elasticity of Fe. Therefore, in our ongoing project we focus on studies of alloy systems at extreme conditions. An example of the results coming from calculations is shown in Fig. 2. Here we use essentially more accurate theoretical treatment of the bcc Fe-Ni alloy at extremely high pressure and temperature as compared with that in Ref. [1], and we confirm our original prediction that the bcc structure becomes dynamically stable.

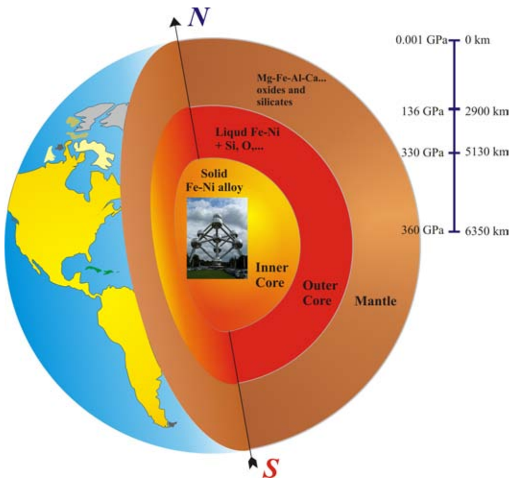


Fig. 1: Schematic view of the Earth's interiors (courtesy by L. Dubrovinsky). The Earth has an outer silicate solid crust, a highly viscous mantle, a liquid outer core that is much less viscous than the mantle, and a solid inner core. Atomium monument placed in the center of the Earth inner core in the figure represents a unit cell of a body-centered cubic (bcc) crystal. In our recent Science publication [1] we showed that it is stable in Fe-Ni alloys at the Earth's core conditions.

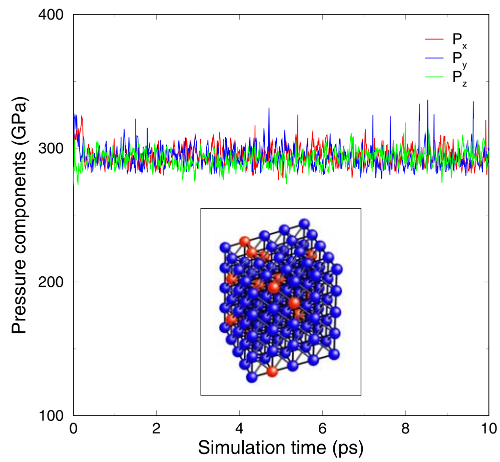


Fig. 2: Results of ab-initio molecular dynamics simulations of Fe-rich FeNi alloy with the bcc crystal structure at 300 GPa and 6000 K. Shown are diagonal pressure components as a function of simulation time. There is no deviation between the average values of the pressure components for x, y, and z-directions. This indicates the dynamical stability of the bcc structure of the alloy, represented by the large supercell with quasi-random distribution of Fe (blue) and Ni (red) atoms (see inset).

Apply for access to HPC capacity

Now it becomes even easier to apply for High Performance Computing, HPC, resources for scientific groups in Sweden. The Swedish National Allocation Committee for HPC, SNAC, doubles the upper limit for allocations on medium level projects on large resources. This will make it possible for more groups to get adequate HPC capacity for their needs through the flexible, quick and comprehensive medium scale application system. In the last application round for large scale allocations a large fraction of the applications would fall into the new sized medium scale category. In this way the application system will be more streamlined, an easier application procedure for the majority of groups and the evaluation can focus stronger on really large applications. The dead-line for large scale applications this autumn is 27 October at 15:00. More information regarding SNAC is available at: http://www.snac.vr.se/.

PETER MÜNGER

In future studies we proceed with extended simulations of the Fe-Ni phase diagram using AIMD, complemented with such powerful computational techniques as thermodynamic integration and global structure optimization to make novel inroads for the enigma of the Earth's interior. We acknowledge fruitful support by the Swedish National Infrastructure for Computing (SNIC) program in general and powerful NSC computing resource Neolith in particular. Theory, experiment, and simulations deeply interconnected in this project will lead further in our voyage to the Earth's deep interior.

A. MIKHAILUSHKIN, S.I. SIMAK AND I.A. ABRIKOSOV

THEORY AND MODELING DIVISION, DEPARTMENT OF PHYSICS, CHEMISTRY AND BIOLOGY, LINKÖPING UNIVERSITY

References

[1] L. Dubrovinsky, N. Dubrovinskaia, O. Narygina, I. Kantor, A. Kuznetzov, V. Prakapenka, L. Vitos, B. Johansson, A. S. Mikhaylushkin, S. I. Simak, and I. A. Abrikosov, "Body-centred Cubic Iron-Nickel Alloy in the Earth's core", Science 316, 1880 (2007).
[2] A. S. Mikhaylushkin, S. I. Simak, L. Dubrovinsky, B. Johansson, and I. A. Abrikosov, "Pure Iron Compressed and Heated to Extreme Conditions", Phys. Rev. Lett. 99, 165505 (2007).
[3] L. Dubrovinsky, N. Dubrovinskaia, F. Langenhorst, D. Dobson, D. Rubie, C. Geshmann, I. A. Abrikosov, B. Johansson, V. I. Baykov, L. Vitos, T. Le Bihan, W. A. Crichton, V. Dmitriev, and H.-P. Weber, "Iron-silica interaction at extreme conditions and the electrically conducting layer at the base of Earth's mantle", Nature 422, 58 (2003).
[4] L. Dubrovinsky, N. Dubrovinskaia, I. Kantor, W. A. Crichton, V. Dmitriev, V. Prakapenka, G. Shen, L. Vitos, R. Ahuja, B. Johansson, and I. A. Abrikosov, "Beating the miscibility barrier between iron and magnesium by high-pressure alloying", Phys. Rev. Lett. 95, 245502 (2005).

Igor Abrikosov received a degree of Doctor of Physics and Mathematics in "Solid State Physics" at Moscow Steel & Alloys Institute (Technological University) in 1997. From 2003 he is Professor in Theoretical Physics at the Department of Physics, Chemistry, and Biology (IFM), Linköping University.

New HPC resources for SMHI and Saab

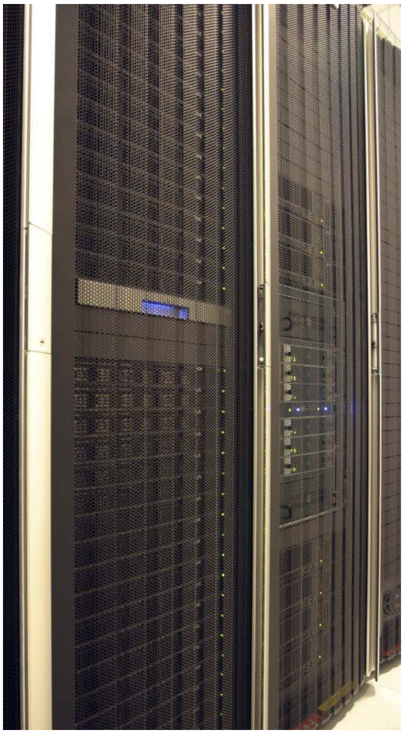
NSC has recently acquired new HPC resources in collaborations with our partners SMHI and Saab. The new clusters are designed by NSC together with our partners in order to arrive at optimal solutions with respect to the users' requirements and price/performance ratio.

For Saab, there is a new Linux cluster, with the name Skylord, consisting of 40 HP ProLiant DL160 G5 servers with two 2.8 GHz quad-core Intel Xeon processors and 16 gigabyte RAM, giving a total of 320 processor cores. The network technology used for application communication is a fast Infiniband DDR (20 gigabit/s). With the new system Saab will be able to make powerful calculations within the areas of airoelastics, fluid dynamics, air turbulence and radar signatures.

For SMHI, there are two new Linux clusters, named Bore and Gimle. Gimle is used for simulation model development and Bore is running the production simulations for weather forecasts. Together the two clusters have 140 servers, also of the HP ProLiant DL160 G5 2.8 GHz quad-core Intel Xeon type, interconnected with fast Infiniband DDR network, configured in a full bisection fat-tree topology. In total, the SMHI systems have a top performance of 12.5 teraflop/s. The new systems will be used for faster and more detailed weather forecasts with much better resolution than earlier.

Furthermore, to meet the demand of network capacity for weather production, model development and climate research, and to prepare for the ever increasing transfers of data volumes, we have established several wavelength-based connections between SMHI and NSC, each currently running at one gigabit per second.

These new acquirements are evident signs of the fruitful collaborations between NSC and our partners SMHI and Saab.



UPCOMING EVENTS

Los Alamos Computer Science Symposium (LACSS) 2008
October 13–15, 2008. Santa Fe, USA.
http://www.lanl.gov/conferences/lacss/2008

NSC'08 conference with focus on storage issues
October 14–15, 2008. Linköping, Sweden.
http://www.nsc.liu.se/nsc08

SUSEC autumn workshop with a focus on security issues
October 14–15, 2008. Linköping, Sweden.
http://www.nsc.liu.se/nsc08

SUNET TREF-punkt 19 with focus on network issues, Linköping University
October 15–16, 2008. Linköping, Sweden.
http://www.nsc.liu.se/nsc08

PACT 2008; 7th International Conference on Parallel Architectures and Compilation Techniques
October 25–29, 2008, Toronto, Canada.
http://www.eecg.toronto.edu/pact

E- science conference: Global Challenges – Regional opportunities: How can Research Infrastructure and eScience support Nordic competitiveness?
November 12–13, 2008, Stockholm, Sweden.
http://www.vr.se

SC 08; International Conference for High Performance Computing, Networking, Storage and Analysis
November 15–21, 2008, Austin, Texas, USA.
http://sc08.supercomputing.org

ICPADS 2008; 14th International Conference on Parallel and Distributed Systems
December 8–10, 2008, Melbourne, Australia.
http://www.deakin.edu.au/conferences/icpads2008

HiPC-08: International Conference on High Performance Computing
December 17–20, Bangalore, India.
http://www.hipc.org

HPCA-15; 15th International Symposium on High-Performance Computer Architecthure
Febr 14–18, 2009, Raleigh, North Carolina, USA.
http://www.comparch.ncsu.edu/hpca

PPoPP 2009; 14th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming
Febr 14–18, 2009, Raleigh, North Carolina, USA.
http://ppopp09.rice.edu

PerCom-09; IEEE Intl Conference on Pervasive Computing and Communications
March 16–20, 2009, Dallas, USA.
http://www.percom.org

HP-Cast NTIG (Nordic Technical Interest Group in HPC using HP clusters)
Preliminary daty: March 24–25, 2009, CSC, Finland.
http://www.csc.fi

IPDPS-09: IEEE International Parallel and Distributed Processing Symposium
May 25–29, 2009, Rome, Italy.
http://ipdps.org

HiCOMB 2009 8th IEEE International Workshop on High Performance Computational Biology
May 25, 2009. Rome, Italy.
http://www.hicomb.org

Linköpings universitet
National Supercomputer Centre, Linköpings universitet, 581 83 Linköping, Sweden
Tel: +46 (0) 13-28 26 18, fax: +46 (0) 13-28 25 35, e-mail: info@nsc.liu.se
www.nsc.liu.se