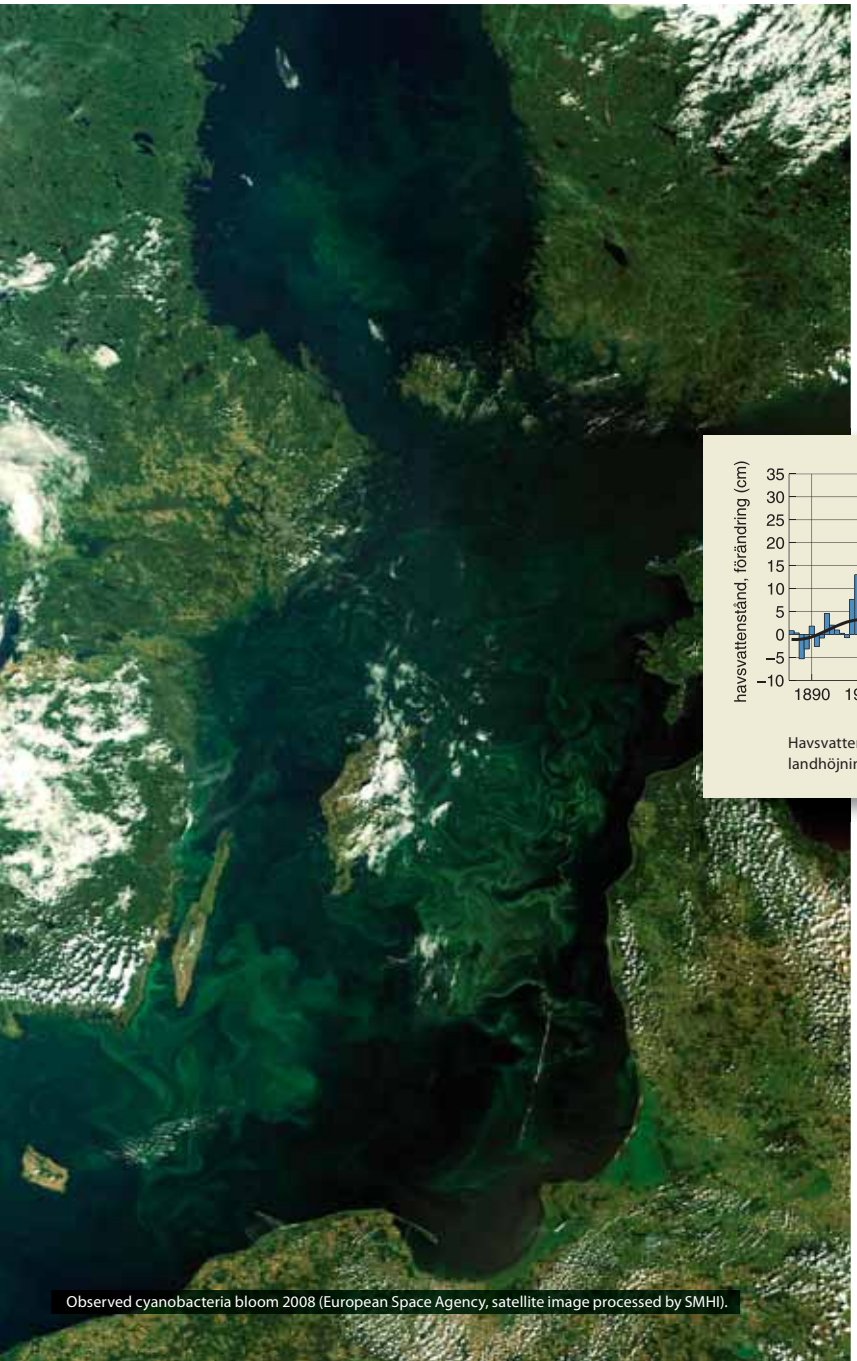
NSC News
National Supercomputer Centre at Linköpings universitet
2010:1

The Baltic Sea ecosystem



Observed cyanobacteria bloom 2008 (European Space Agency, satellite image processed by SMHI).

Impact of changing climate on the marine ecosystem of the Baltic Sea

The Swedish Meteorological and Hydrological Institute (SMHI) is leading an international effort to calculate the combined effects of changing climate and changing nutrient loads on the Baltic Sea ecosystem.

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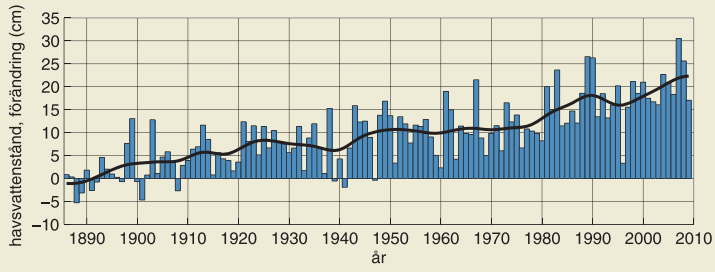

Havsvattenståndets förändring för 13 svenska mareografer sedan 1886 där effekten av landhöjningen tagits bort (källa SMHI).

Capacity computing at NSC

NSC has recently acquired a new HPC resource named Kappa.

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More computers, more personnel, and more e-science

Now when spring is approaching after a long winter, it also means spring-time for computers at NSC. Our new capacity system, kappa, is up and running, and more and more users will now get access to that system. It fills an important niche in the computational ecosystem at NSC in providing a suitable resource for pleasantly parallelisable tasks. It will also add important computational capacity for all users, both locally and nation-wide. For our collaboration with SMHI, a new system is on its way. Furthermore, we will soon set up the dedicated resource "matter" for material science, funded by the Knut and Alice Wallenberg foundation, but more about that in next issue of NSC News.

We cordially welcome two new system administrators to NSC – Andreas Johansson and Mats Kronberg – who will contribute valuable knowledge and increase our operational capacity when we now are expanding both on the calculation side and on the storage side. Please read their more detailed presentations in this issue.

NSC has substantially improved our internet connections, now having 10 Gbit/s connectivity. This capacity is needed to serve the steadily increasing data transfer of all users and for back-up between SNIC centres. More about this in a separate article.

The Swedish e-Science Research Centre, SeRC, one of the new strategic research areas, will stimulate increased interactions between high-performance computing centres such as NSC and scientists heavily using computational methods in their research. SeRC will support development of new methods and increase the efficiency of computer utilisation in research. SeRC covers a wide range of e-science application areas, of which seven are initiated during 2010: bioinformatics, complex diseases, electron structure, flow, particle simulation, visualisation and numerical analysis. SeRC will arrange a kick-off on 22 – 23 April with all SeRC groups and internationally invited experts in e-science that will contribute to interesting discussions, important planning and facilitation of cross-disciplinary contacts. SeRC has already started the recruitment process, where several faculty positions will be announced at Linköping University, Royal Institute of Technology, Stockholm University and Karolinska Institutet. Furthermore, there will be additional application experts to help NSC users with optimisation of programs for parallel processing and testing, installing and tuning of scientific software. NSC will announce a number of such positions during the year.

Finally, I would like to wish all NSC users a fruitful spring with increased computational possibilities in various fields.

BENGT PERSSON, NSC DIRECTOR

NSC Network Upgrade

On February 17, we upgraded our connection between NSC's two routers and the Linköping university backbone from 1 to 10 gigabit/s. The university had then already upgraded its SUNET connection to 10 gigabit/s.

Most NSC systems are still connected via 1 gigabit/s ports and will be upgraded as needed in the future, but they already benefit from the upgraded connection as several system may together use more than 1 gigabit/s towards the Internet.

Incidentally, this is not NSC's first 10 gigabit/s connection. Since last summer, NSC (as well as PDC and HPC2N) has a 10 gigabit/s connection to the LHC-OPN (use for traffic related to the CERN experiments).

KENT ENGSTRÖM

New staff member: Andreas Johansson

Born on the Swedish west coast, I moved to Linköping in 1993 to study for a masters degree in Computer Science and Engineering, and has been here since then. Although this is my first HPC related employment, I've been working as a Unix systems and network administrator since 1998. Prior to NSC I worked for seven years at the Department of Computer and Information Science at Linköping University, so I'm familiar with the academic environment. At NSC I will mostly be working with administration of the SNIC computational resources.

Impact of changing climate on the ma

In November 2007 the ministers responsible for environment of all Baltic Sea countries signed a remarkable document, the Baltic Sea Action Plan (BSAP), initiated by the Helsinki Commission (HELCOM, see http://www.helcom.fi). According to this plan nutrient loads into the sea should significantly be reduced. Each country will contribute with its own specific share to reduce the enhanced nutrient concentrations (eutrophication) in the Baltic Sea caused by high population density and intensive agriculture in the region. During recent decades eutrophication-associated problems like oxygen deficiency in the deep water, spreading of dead bottom zones, increased frequency and intensity of blue-green algae blooms, etc. are believed to be the most severe threats to the Baltic Sea ecosystem.

As the response of the Baltic Sea is slow and an improved state is not expected to occur before several decades after the implementation of the BSAP, changing climate has to be taken into account. Nutrient load reductions might not have the same effect in future climate than in present climate. Within a recently performed assessment of climate change for the Baltic Sea basin it was concluded that global warming may cause hydrographic changes that may have significant impacts on the marine ecosystem and its biodiversity [1].

Today the Swedish Meteorological and Hydrological Institute (SMHI) is leading an international effort to calculate the combined effects of changing climate and changing nutrient loads on the Baltic Sea ecosystem. 11 partners from 7 Baltic Sea countries are contributing to this three-year (2009 – 2011) project called ECOSUPPORT (Advanced modeling tool for scenarios of the Baltic Sea ECOsystem to SUPPORT decision making, http://www.baltex-research.eu/ecosupport). Within ECOSUPPORT the so-called dynamical downscaling approach is applied to calculate the future climate of the Baltic Sea using a high-resolution coupled atmosphere-ice-ocean-land surface regional climate model, the Rossby Centre Atmosphere Ocean Model (RCAO), with lateral boundary data from coarser resolution global climate models (GCMs) (Fig.1).

To assess uncertainties of scenario simulations related to the natural variability, unknown future greenhouse gas emissions, unknown future nutrient loads to the sea, and biases of the models, an ensemble of regional scenario simulations is performed. In difference to earlier studies addressing selected time slices [1], the new scenario simulations are transient simulations covering the whole period 1961 – 2099. Thus, limiting assumptions on the changes of the high frequency variability are not necessary.

The results of the RCAO scenario simulations are used to force integrated system models of the atmospheric, land surface and marine biogeochemistry and marine food web models (including higher trophic levels like fish and seals). These models add complexity with additional variables, higher horizontal and vertical resolution but also with higher computational demands. To estimate uncertainties related to the description of some key biogeochemical processes a multi-model ensemble consisting of three coupled physical-biogeochemical models for the Baltic Sea are used within ECOSUPPORT to estimate the impact of climate change on the marine ecosystem [2]. The marine biogeochemical models are used to calculate changing concentrations of nitrate, ammonium, phosphate, diatoms, flagellates, cyanobacteria, zooplankton, detritus, and oxygen in the Baltic Sea [3].

For present climate 1961 – 2007 the RCAO model results forced with GCMs are compared with available observations. Mean seasonal cycles of important parameters like 2m air temperature over the Baltic Sea are

Fig.1. Model domain of the Rossby Centre Atmosphere Ocean model (RCAO) covering most of Europe and parts of the North Atlantic Ocean and Nordic Seas. Only the Baltic Sea is interactively coupled.

New staff member: Mats Kronberg

I have just joined NSC as a systems expert on distributed computing. Initially my primary task will be to help take care of Neolith while the primary system administrator is on leave. My background includes ten years at Saab in Linköping, maintaining computer systems for flight simulation and associated software development. More recently I have worked at Opera Software, managing the server clusters for Opera Mini. In scale these are similar to a fairly large HPC cluster, but has a different set of problems, among which are 24/7/365 operations and managing an exponential growth of 10 – 20% per month.

arine ecosystem of the Baltic Sea

well simulated by RCAO when lateral boundary data from especially two selected GCMs are used: HadCM3 from the Hadley Centre in the UK [4] and ECHAM5 from the Max-Planck-Institute for Meteorology in Germany [5].

From the latest scenario simulations two examples are shown in Figures 2 and 3. For the end of the 21st century the model results indicate that the largest warming of the water temperature may occur in the northern Baltic Sea during summer as a consequence of the shortened sea-ice season (Fig.2). Assuming a medium greenhouse gas emission scenario (A1B) the sea surface temperatures may increase in the northern Baltic by up to 4 or 6°C depending on the choice of the forcing GCM. Smallest water temperature changes are projected for the winter season.

As in warmer water the concentration of oxygen saturation is lower, the oxygen concentrations in coastal waters will be reduced in future climate (Fig.3). Consequently, also the deepwater oxygen concentrations will decrease assuming that nutrient loads from land will only alter according to volume flow changes. However, in both GCM driven simulations there are also small bottom areas located on the slopes of the Gulf of Finland, northern Baltic proper, Bothnian Sea and Bothnian Bay with improved oxygen concentrations. The scenario simulations indicate that the runoff increases and the salt water flow from the North Sea into the Baltic Sea decreases causing a reduced stability in the depth of the largest vertical salinity gradient. Due to the reduced stability in this depth more oxygen will be mixed from the surface

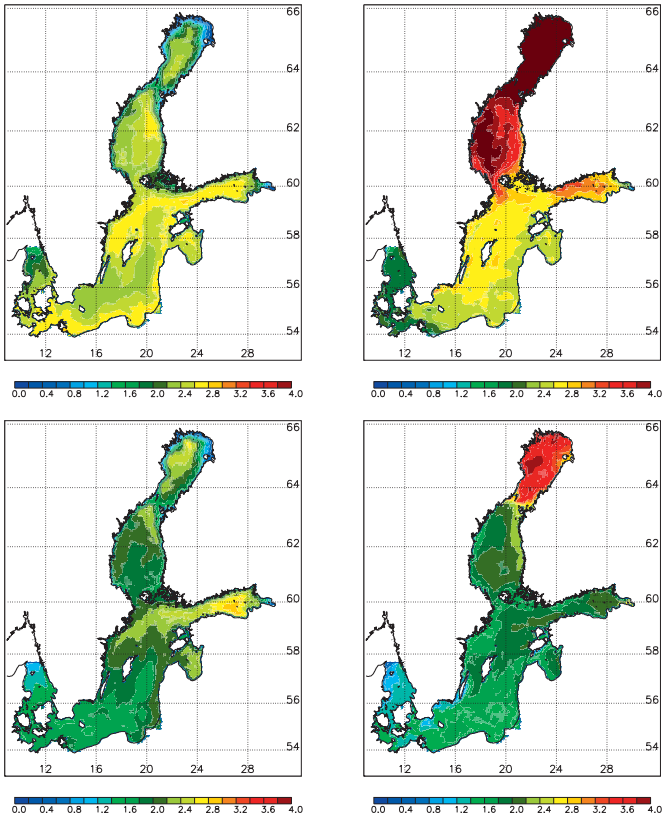

Fig.2. Winter (December to February, left panels) and summer (June to August, right panels) sea surface temperature changes (°C) between the time slices 2060 – 2089 and 1970 – 1999 forced with RCAO/HadCM3 (upper panels) and RCAO/ECHAM5 (lower panels) in the A1B emission scenario.

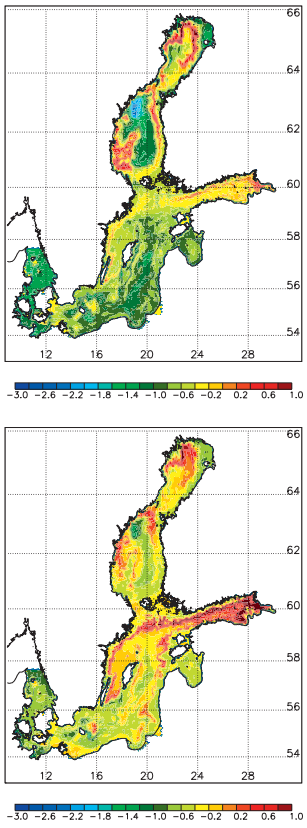

Fig.3. Summer (June to August) mean bottom oxygen concentration changes (in ml/l) between the time slices 2060 – 2089 and 1970 – 1999 forced with RCAO-HadCM3 (upper panel) and RCAO-ECHAM5 (lower panel) in the A1B emission scenario. For the depicted results concentrations of nutrient loads from land are assumed to be unchanged.

down to the bottom. The projected hydrographic and oxygen concentration changes could have significant impacts on the Baltic Sea ecosystem and its biodiversity.

In summary, the objectives of the described research are to calculate the combined effects of changing climate and changing human activity (nutrient load changes from land and air, coastal management, fisheries) on the Baltic Sea ecosystem, to assess the resulting socioeconomic impacts, and to support decision makers and stakeholders with a tool providing them with relevant and readily accessible information that will help to raise wider public awareness.

The expected outcome is an advanced modeling tool for scenario simulations of the whole marine ecosystem that can underpin and inform management strategies to ensure water quality standards, biodiversity and fish stocks.

Financial support from the Swedish Environmental Protection Agency (NV), the Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning (FORMAS), and the European Commission within the BONUS+ program (http://www.bonusportal.org) is gratefully acknowledged. Model simulations were partly performed on the climate computing resources 'Tornado' and 'Ekman/Vagn' funded by grants from the Knut and Alice Wallenberg foundation.

MARKUS MEIER

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Markus Meier is associate professor in physical oceanography, head of the oceanographic research unit at SMHI and adjoint lecturer at the Department of Meteorology at Stockholm University. Especially, he is interested in climate change impact studies of the marine environment with focus on the Baltic Sea and Arctic Ocean.

Capacity computing at NSC

NSC has recently acquired a new HPC resource named Kappa. Kappa is funded by Swedish National Infrastructure for Computing (SNIC) and Linköping University and is intended for general purpose capacity computing. About half of the system will be available for SNIC projects. Swegrid projects will also use a fraction of the Kappa system, providing a more integrated environment for SNIC users.

Intel's Nehalem micro-architecture used in Kappa's processors provides far better memory bandwidth than earlier Intel core architectures. Even if Kappa provides slightly less theoretical flops per core than Neolith, the performance is over twice per core on many applications. However, we still recommend to target applications that scale well towards NSC's large capability cluster, Neolith, and its more powerful Infiniband network.

Kappa is a cluster of 338 servers with two Intel Xeon E5520 processors in each server. There are, in total, 2704 cores available for computing. 56 servers is equipped with 72 gigabyte of memory, all others have 24 gigabyte of memory. In addition to a general purpose gigabit Ethernet, servers are connected to a DDR Infiniband interconnect with reduced bisection bandwidth. Kappa shares disk storage with Neolith. This will become a common storage space for SNIC projects at NSC in the future.

The user environment on Kappa is very similar to that on Neolith. We try to keep the differences to where it really matters. For MPI we currently have OpenMPI as the default but we are evaluating Intel MPI and also Voltaire's accelerated OpenMPI together with their Unified Fabric Manager.

Kappa is built in four encapsulated units where each unit includes two racks of servers, fans and a heat exchangers. Water pipes from the heat exchangers are connected to the district cooling system at Campus. Kappa is manufactured by Hewlett-Packard and delivered by GoVirtual Nordic AB. It was purchased in collaboration with three other SNIC centers: UPPMAX (Uppsala), C3SE (Chalmers), Lunarc (Lund).

NICLAS ANDERSSON

UPCOMING EVENTS

5th EGEE User Forum
April 12 – 15, 2010. Uppsala, Sweden.
http://egee-uf5.eu-egee.org

IPDPS 2010; 24th IEEE International Parallel & Distributed Processing Symposium
April 19 – 23, 2010. Atlanta, Georgia, USA.
http://www.ipdps.org

HEPIX Spring 2010 Meeting
April 19 – 23, 2010. Lisbon, Portugal.
http://www.lip.pt/hepixspring2010

CCGrid10; 10th IEEE International Symposium on Cluster Computing and the Grid
May 2010, Melbourne, Australia.
http://www.gridbus.org/~raj/ccgrid

DEISA PRACE Symposium 2010
May 10 – 12, 2010, Barcelona, Spain.
http://www.deisa.eu/news_press/symposium

Euro-Par 2010; Aspects of Parallel Computing and Distributing Computing
August 31 – September 3, 2010, Ischia, Naples, Italy.
http://www.europar2010.org

PACT; 19th International Conference on Parallel Architectures and Compilation Techniques
September 11 – 15, 2010, Vienna, Austria.
http://www.pactconf.org

ICPP2010; 39th International Conference on Parallel Processing
September 13 – 16, 2010, San Diego, CA, USA.
http://www.cse.ohio-state.edu/~lai/icpp2010

IEEE Cluster 2010
September 20 – 24, 2010. Heraklion, Crete, Greece.
http://www.cluster2010.org

LISA'10; 24th Large Installation System Admininstration Conference
November 7 – 12, 2010, San Jose, CA, USA.
http://www.usenix.org/event/lisa10

SC10; International Conference for High Performance Computing, Networkng, Storage and Analysis
November 13 – 19, 2010, New Orleans, LA, USA.
http://sc10.supercomputing.org

ICPADS 2010; 16th International Conference on Parallel and Distributed Systems
December 8 – 10, 2010, Shanghai, China.
http://grid.sjtu.edu.cn/icpads10

HiPC2010; International Conference on High Performance Computing
December 19 – 22, 2010, Goa, India.
http://www.hipc.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

Editor: Peter Münger To subscribe, for a paper version and/or PDF-file, send an email to info@nsc.liu.se