NSC News 2007:2
National Supercomputer Centre at Linköpings universitet

A New System

Right now, NSC is taking delivery of the first components of a supercomputer cluster that will eclipse anything seen before in Sweden.

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Modelling the Climate

Markku Rummukainen and Erland Källén describe how computer modelling can help predict climate changes.

Read further on page 3

Capability resource

Sven Stafström
NSC Director
stafstrom@nsc.liu.se

It was indeed an exciting and happy moment when we could announce the procurement of our new capability resource. The system, which is presented in detail below, has been financed by SNIC and is delivered by Go Virtual Nordic AB and Hewlett-Packard. When it is accepted in October it will be, by far, the most powerful system available to the academic users in Sweden. The first part of the system has already been delivered when you read this and we might even have performed the first test runs on the system. Some time during summer we will invite pilot users to run on the system – could this be a reason to delay your summer vacation?

I would like to take this opportunity to thank, first of all, SNIC for financing the new system, it was indeed a generous support we received and we have done our best to convert the currency into the best possible hardware solution. Special thanks also to the NSC staff that did all the work; Niclas Andersson has been the project leader and responsible for most of the interactions with the vendors, Peter Kjellström and Mattias Slabanja provided the input to the design of the system and evaluated the solutions proposed by the vendors, and Torgny Faxén and Patrick Norman, together with Mattias, performed the benchmarks test. We are now looking forward to the collaboration with Go Virtual and Hewlett-Packard to reach the common goal to provide our users with a top class resource.

In parallel with the installation of the first part of the capability resource, we are also admiring the skilful construction work that will result in our new computer building. From the outside it looks almost completed by now, but much remains to be done to turn the large hall into a computer room. As a consequence of the construction work we will be forced to turn off the electricity altogether three times, the first turn off has already passed and the two remaining will be announced at least a week in advance. We are sorry for the inconvenience these power cuts cause our users, everybody involved are doing their best to keep the down periods as short as possible.

The feeling of summer came early this year but it will take some time before we can fully enjoy it. Anyway, this is the time to wish all readers of NSC News a nice and relaxing summer holiday.

NSC's 60 Tflops Cluster

This autumn, NSC will be able to present a supercomputer with a computing power unprecedented in Sweden.

In NSC's new computer building, 805 compute nodes will form a cluster with a theoretical peak speed of 60 teraflops. In addition to being the most powerful supercomputer in Sweden, it will rank highly on the Top500 list of the world's fastest computers.

The compute nodes are HP ProLiant DL140 G3 with two Quad-Core Intel® Xeon® E5345 processors each. In addition, the system will contain five ProLiant DL380 G5 system servers. The total main memory size of the system is 14 terabytes, with 90% of the nodes being equipped with 16 gigabytes of memory and 10% with 32 gigabytes. The nodes communicate over a high-speed network based on Cisco® Infiniband equipment, providing an aggregate bandwidth exceeding 32 terabits per second.

The system is delivered by Go Virtual and HP, and is funded through a grant from SNIC, Swedish National Infrastructure for Computing.

The system will be brought into production gradually during the summer and autumn.

LCSC

Linux Clusters for Supercomputing
Linköping October 16–18, 2007

Keynote: Dr. Horst Simon

Technical programme • Tutorials • Inauguration of the new 60 Tflops cluster

Climate Modelling

Climate change is a major environmental and socio-economic challenge. What makes it special is its anticipated impacts, global nature and the long lead times between cause and effect. Climate change also links to many other burning environmental and socio-economic issues.

The overall cause and effect, mechanisms and implications of anthropogenic climate change are reasonably well understood. The growth of anthropogenic greenhouse gas emissions (the forcing) changes atmospheric composition and enhances its greenhouse effect. The climate system responds by warming up at the surface and in the lower atmosphere (and by a cooling in the upper atmosphere). The warming initiates melting of sea ice and mountain glaciers, an increase in the heat content of the surface ocean, a sea level rise, as well as other changes. Some of these feed back to climate change by means of interactions in the biogeophysical climate system. Many give rise to impacts.

Uncertainties

Whereas the mechanisms of climate change are well understood, some of the details are much less so. We know that the climate system sensitivity (a measure of how much climate will change for a given amount of forcing) is significantly different from zero, but it has proven notably difficult to nail down. This is especially true to its upper limit. (The higher the value, the larger is the expected change for a given amount of forcing.) This uncertainty is due to uncertainties in the feed back mentioned above within the climate system, involving clouds, the carbon cycle and physical ocean processes. Another uncertainty is that little can still be said about various large-scale non-linear responses of the climate system to continued forcing. During natural climate forcing episodes far back in time, such occurrences are found. A few other aspects of uncertainty concern how the occurrence of extreme weather events will be altered and how large-scale circulation systems might reorganise, and either add to or reduce the general warming etc. tendencies in different regions.

Some of the uncertainty is inherent and will never totally go away. Perfect knowledge of the momentary state of the complex climate system, which would be required to initialise perfect projections (given perfect models), will always elude us. A numerical representation of the climate system will always fall short of the real thing. Especially the former aspect is due to lack of empirical data. The latter shares some of this, but is also due to a lack of sufficient computing capacity.

Computing capacity

Climate modelling is a challenge even for today's computing capacity. This has to do with the terrific range of spatial and temporal scales. (In size: from planetary circulation systems to molecular dissipation of kinetic energy and to energy transitions within an atom; in time: from millennia to a fraction of a second.) The fundamental hydromechanical equations of the flow

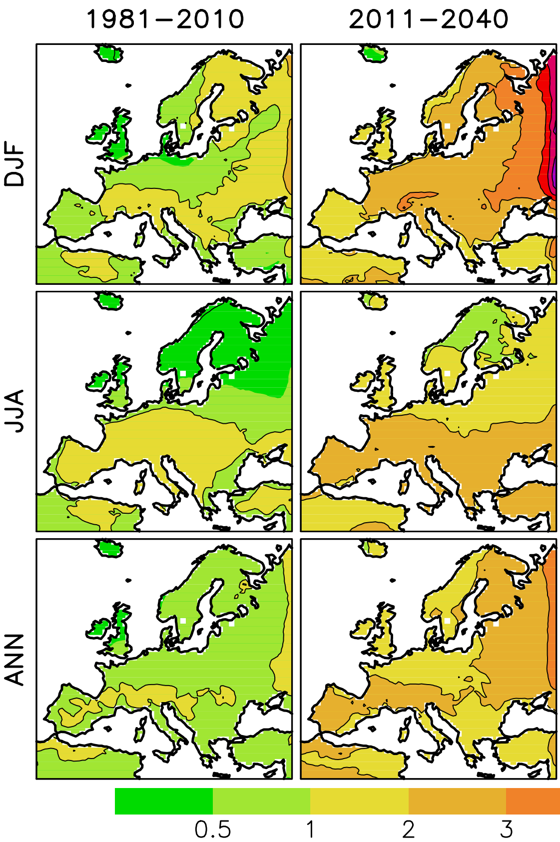
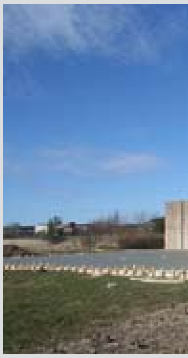


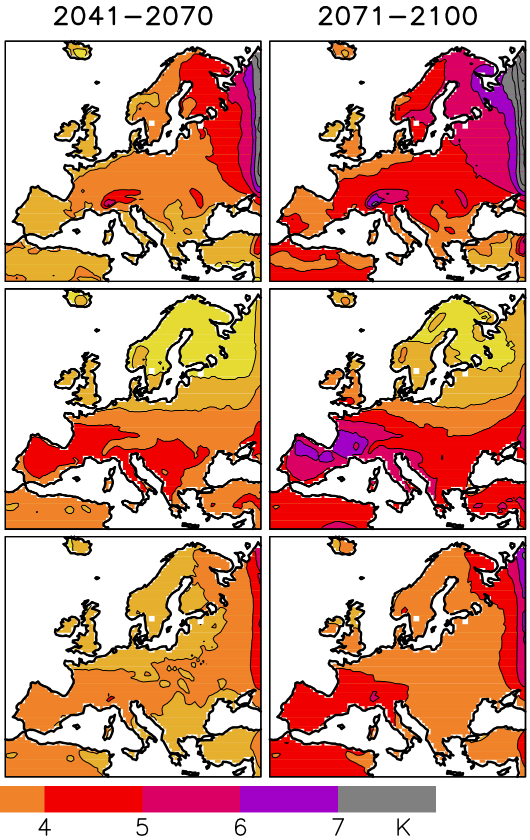
Figure A. An example of simulated regional seasonal (winter, summer) and annual m… Rossby Centre regional climate model RCA3, one of the IPCC SRES emission scenario… been made as a continuous calculation with a time step of around 30 minutes, throu… that a non-linear. See Kjellström et al., 2005, SMHI RMK No 108.

The New Computer Building

NSC's new computer building is rapidly taking shape. In just a few weeks the construction site has been transformed from a muddy playground for excavators to a building that looks finished from the outside.

However, much work remains before the building can house NSC's new main system. Not only must the interior structure be built, and cooling, electrical and network equipment be installed – the electrical system of the entire campus must be upgraded!





ean temperature changes, shown for successive 30-year periods, based on the
s and an ECHAM4/OPYC3 global climate model simulation. The simulation has
gh the period 1961-2100. There are also changes in the variability and extremes

in the atmosphere and the ocean also constitute a non-linear system, in which small inaccuracies can lead to unexpected alterations. Thus, there is a call for computing capacities sufficient for many and yet more simulation variants, such as ensembles, to explore related uncertainties.

Climate models come with different levels of complexity and can be either global or regional. High resolution increases the possibility for an increasingly faithful representation of the processes and non-linearity. It relaxes the need to rely on approximations (parameterisations of physical processes) and thus can decrease structural model uncertainty. Increasing resolution is, however, expensive – halving the grid size leads to an 8 to 16 fold increase in computing, and also increases data output. Of Swedish climate modelling efforts at the Rossby Centre and Stockholm University, much has been on regional climate models for Europe and the Nordic region. For us, the past decade has witnessed increases in resolution (from around 100km to around 25km), incorporation of new model components (such as vegetation component, in collaboration with Lund University) and more/longer regional climate projections (from 30-year long "time slices" to transient 140-year simulations. One example of the newer long runs is given in Figure A). Advances have been possible thanks to increases in computing resources. We have over the years worked on a variety of platforms hosted by NSC, including the Cray C90, T3E, SGI3k, Monolith and, most recently, Tornado, funded with a grant from the Knut and Alice Wallenberg foundation.

New resources

Earlier this year, we were granted together with KTH 20 MSEK by the Knut and Alice Wallenberg foundation and SNIC for a dedicated fluid and climate dynamics computer. The new resource might approach 60 Tflop/s in peak performance and have a mass storage system in excess of 200 Tb. This will provide unprecedented opportunities for our climate modelling. We will be able to work on a comprehensive Earth System Model with interactive vegetation, chemistry, carbon cycle and ice sheets; to increase model resolutions and the number of simulations, and to look into earlier unapproachable scientific issues.

Why a dedicated resource? As already alluded to, the climate system is tightly coupled across a terrific range of spatial and temporal scales. The nature of the interactions is such that the problem is notoriously impossible to break down to smaller pieces. Climate modelling requires computers with fast interconnect and low latency, i.e. capability architectures, and can not be efficiently run on present-day grid computing systems.

Another special facet of climate computing is data output. This depends on the scale and resolution of the particular model, but a relatively high resolution climate simulation, with reduced set of output, leads to a few TB of data

in need of archiving. These need to be effectively kept track of, retrieved, analysed and visualised. Here data grids can offer advantages, alternatively a mass storage system interfaced on a capability computer.

The research into remaining key uncertainties on climate change requires substantial computing power. During the next decade, climate models will certainly gain this, and will subsequently be developed further in terms of process descriptions and resolution. Additional demand on more computing power is exerted by the need to pursue extended-length climate simulations, in larger numbers, to sample natural variability, extreme events and any non-linear behaviour of the system. The expected increase in model resolution is from today's 100-200 km globally and 50 km regionally to 10-50 km and 1-10 km, respectively.

The computational challenges on climate model science include:

(i) Increased spatial resolution: To simulate cloud dynamics, a spatial resolution of 1km or less is required, which is far beyond present capacities. Important elements of ocean circulation also have finer spatial scales than those explicitly resolved in present models;

(ii) New model components (see above);

(iii) Simulation length: The long timescales involved in climate-ocean-glacier-carbon cycle interactions are important in the past and future climate states. To map long-term consequences such as the fate of the great ice sheets and other switch and choke points in the Earth System.

(iv) Ensemble Runs: Inter-model and intra-model ensemble sizes need to increase from a few tens to several hundreds.

These amount up to quite a few orders of magnitude when it comes to additional computing resources, and will keep us busy in the years to come.

Markku Rummukainen is associate professor in meteorology at Helsinki university and has been Head of Rossby Centre, the SMHI climate modelling research unit in Norrköping, following directorship of the Swedish regional climate modelling programme SWECLIM in 2000-2003. He has also worked on global atmospheric chemistry modelling.

Erland Källén is professor in dynamic meteorology at Stockholm university.

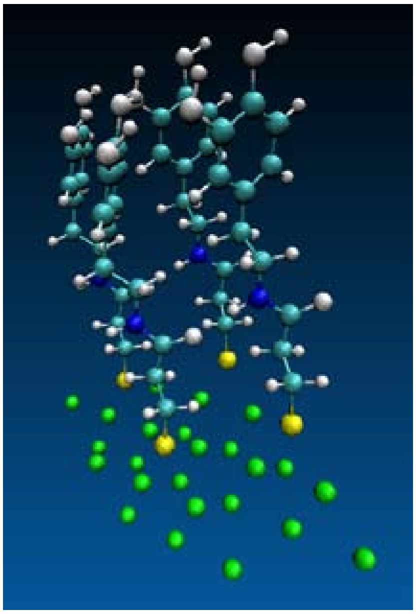
Visualization service at NSC

NSC starts a visualization service available to our SNAC users. This unique service is predominantly concerned with the visualization of molecular and crystal structures as well as electron densities. During the last decade we have seen a rapid increase in the amount of software serving as graphical user interfaces to various electronic structure programs.

With the current initiative, NSC provides access to our supercomputers from a common and dedicated visualization server named Inspector, that collects graphical software for the interaction with the set of electronic structure programs available on our resources. It is our sincere hope that many of our users will find this new service useful and make computational research at NSC easier and even more fruitful.

As member of an active SNAC project you are welcome to request an account on Inspector by sending an e-mail to support@nsc.liu.se.

You may learn more about our new service from our homepage: http://www.nsc.liu.se/software/visualization/



An illustration of a Vasp input file using the graphical user interface named Visual Molecular Dynamics, which is available on Inspector.

UPCOMING EVENTS

International Summer School in Grid Computing

July 8–20 2007, Mariefred, Sweden.
http://www.iceage-eu.org/issgc07/

HLRS; 1st Parallel Tools Workshop

July 9-10 2007, Stuttgart, Germany
http://www.hlrs.de/news-events/events/2007/tools_ws/

PASCO 2007; Parallel Symbolic Computation

July 27–28, 2007. London, Canada.
http://www.orcca.on.ca/conferences/pasco2007

Euro-Par 2007; The 13th International European Conference on Parallel and Distributed Computing

August 28–31, 2007, Rennes, France.
http://europar2007.irisa.fr/

PaCT-2007; Parallel Computing Technologies

September 3–7, 2007. Pereslavl-Zalessky, Russia.
http://www.ssd.sscc.ru/conference/pact2007/

Workshop on High-Performance Computing

September 3–4 2007, Zürich, Switzerland.
http://people.inf.ethz.ch/cflaig/hpc07/

ParCo2007; Parallel Computing 2007

September 4–7, 2007. Juelich and Aachen, Germany.
http://www.fz-juelich.de/parco2007/

ICPP 2007; 2007 International Conference on Parallel Processing

September 10–14, 2007. XiAn, China.
http://www.cse.ohio-state.edu/~icpp2007/

The 8th IEEE/ACM International Conference on Grid Computing (Grid 2007)

September 19–21, 2007. Austin, Texas, USA.
http://www.grid2007.org

24th IEEE MSST2007 Conference on Mass Storage Systems and Technologies

September 24–27, 2007. San Diego, CA, USA.
http://storageconference.org/2007/

IEEE Cluster2007

September 17–21, 2007, Austin, Texas, USA.
http://www.cluster2007.org/

Grid 2007; The 8th IEEE International Conference on Grid Computing

September 19–21, 2007, Austin, Texas, USA.
http://www.grid2007.org/

EuroPVM/MPI 2007; The 14th European PVM/MPI Users's Group Conference

September 30–October 3, 2007, Paris, France.
http://pvmmpi07/lri.fr/

EGEE'07; Enabling Grids for E-SciencE

October 1–5, 2007, Budapest, Hungary.
http://www.eu-egee.org/egee07/home.html

I-SPAN 2007; The 9th International Symposium on Parallel Architectures, Algorithms and Networks

October 11–13, 2007, Sydney, Australia.
http://www.it.usyd.edu.au/~ispan07/

LCSC 2007; The 8th Annual Workshop on Linux Clusters for Super Computing

October 16–18, 2007, Linköping, Sweden.
http://www.nsc.liu.se/lcsc

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.

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