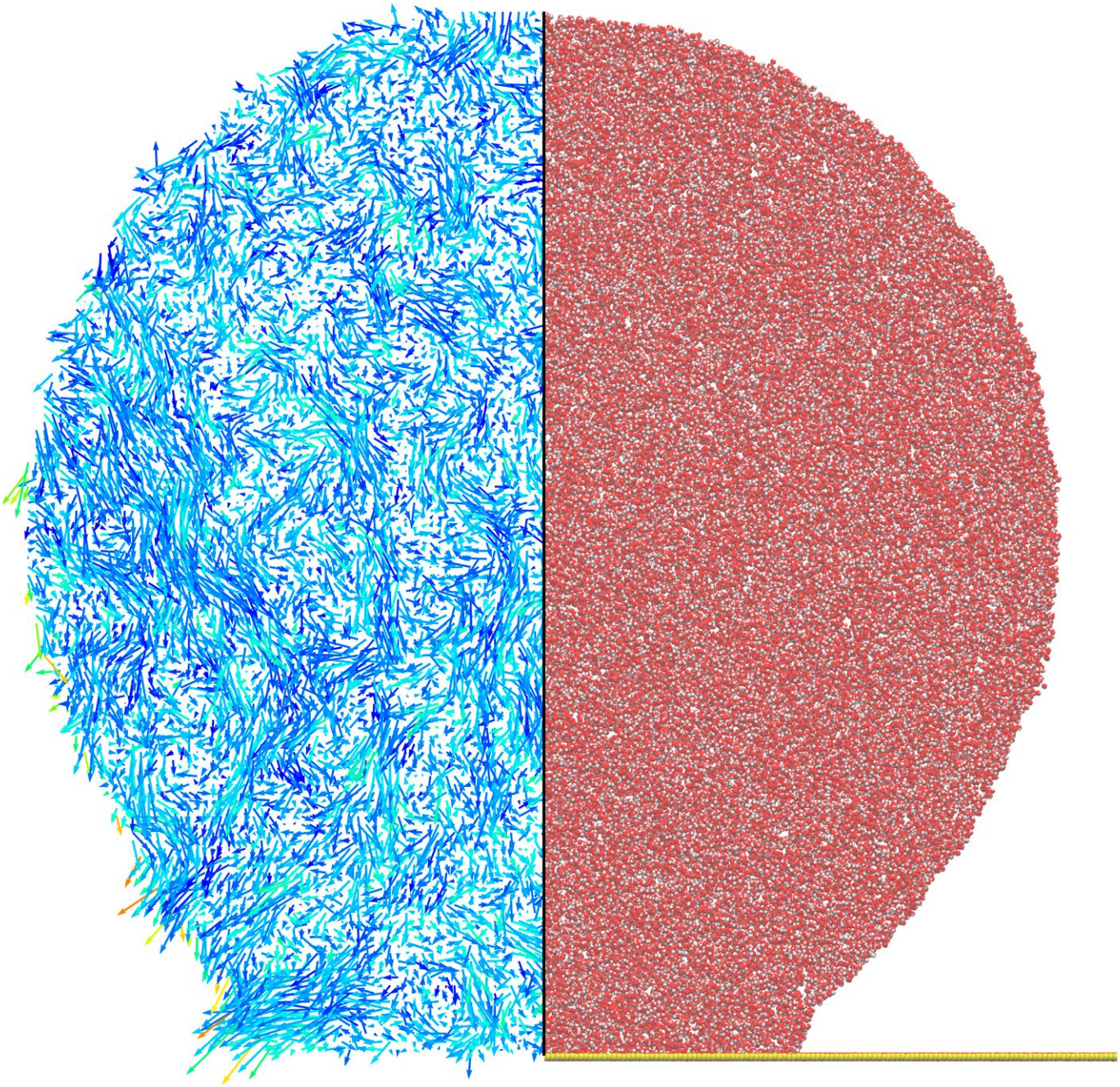
SeRC
Swedish e-Science Research Centre

News

2014:1



Evaluating the first five years of SeRC

Cover: In a new collaboration, the SeRC Molecular simulation and FLOW communities have performed the largest simulations of water droplets to date, which spans the length scales from atomistic to fluid dynamic descriptions. Image by Petter Johansson and Berk Hess.

The first five years of SeRC and the self-evaluation

SeRC has now existed for almost five years, and in May 2015 the Swedish Research Council will report to the government regarding SeRC and the other 42 Strategic research areas. This will be based on a self-evaluation earlier this year, and in December 2014 hearings will be conducted with an international expert panel. This fourth newsletter will be devoted to what we have done during the first five years, both in terms of scientific results and building SeRC as a platform including research, infrastructure and computer experts.

"SeRC-groups are cited 77% more than the mean rate in the field"

SeRC has generated ground-breaking results with very high impact in important e-Science areas by forming strong communities and collaborations involving both core technology and applications, and some of the results are summarized in this issue. The success is reflected in our publication output, which increased by 50% from 2010 to 2013, and we have a number of works in Nature, Science, and top-ranking journals of each field – several by younger faculty recruited as part of the SeRC initiative! Considering the SeRC financing is a small part of the total funding this is a strong indication of well-working synergy effects. In addition, SeRC researchers had an average field normalized citation rate of 1.77 during 2010–2012, which means that publications from SeRC-groups are cited 77% more than the mean rate in the field. You can read about some of our scientific highlights in this issue of the newsletter and more information can be found at http://www.e-science.se/results.

We have built an organization that enables the multidisciplinary collaborative research that e-Science consists of, and initiated collaborations between the large computer centers at KTH (PDC) and Linköping (NSC) with 80% of Swedish resources. There is now a MoU signed by the presidents, and the centers participate in each other's board meetings.

We took the initiative to organize the new advanced application experts (AEs), which SeRC coordinates nationally in collaboration with SNIC, and we have made strategic worldwide recruitments of 12 highly skilled assistant professors, that now takes part of the SeRC faculty.

"We took the initiative to organize the new advanced application experts (AEs), which SeRC coordinates nationally in collaboration with SNIC"

The SeRC faculty is a core group of researchers that are involved in the formation of the SeRC strategy together with the Steering board. They have also engaged in team-building activities together with our application experts. Further, in 2012/2013 we performed an internal evaluation where we, among other things, happily discovered more than 30 collaborations between different SeRC groups; and with application experts. In December 2013, to consolidate the organization, SeRC turned into a research center with KTH as host, and we have now recruited an external chair of the board, Prof. Morten Dæhlen, Dean of Mathematics and Natural Sciences at the University of Oslo and a prominent international e-Science leader.

"we have made strategic worldwide recruitments of 12 highly skilled assistant professors"

More than 70 publications in SeRC involve collaborations with industry and agencies, which is outstanding considering our fundamental research focus. SeRC has developed software with impact on several sectors, ranging from life science and visualization to aeronautics and lighting, and we have introduced e-Science methodologies within a wide range of societal sectors through direct collaborations with agencies, and by raising public awareness. You can read more about our collaborations in this issue of the newsletter, like the SeRC-STHLM3 collaboration, where e-Science tools are used to evaluate population-based prostate cancer screening tests, or our contribution to computing resources to the studies assessed by the latest intergovernmental panel on climate change (IPCC). More information can also be found at http://www.e-science.se/industry. SeRC has also influenced research policy by contributing several panel members and the chair, Anders Ynnerman, to the Swedish Research Council's report on "Swedish Science Cases for e-Infrastructure" (http://www.e-science.se/news/swedish-science-cases). We have also taken a high profile concerning e-Science and Big Data in health care, most recently through our annual conference at Karolinska Institutet (http://www.e-science.se/annualmeeting2014).

"More than 70 publications in SeRC involve collaborations with industry and agencies"

Last but not least, many SeRC researchers have raised public awareness in numerous interviews and seminars, including a large SeRC event with the 2013 Chemistry Nobel Laureates, and SeRC researchers were the scientific partners for the national television programs on the prize. SeRC researchers have also made a large number of presentations at schools and museums, and SeRC results are shown in exhibits and presentations at the Visualization Center C in Norrköping, with over 100,000 visitors per year. It is a core mission of SeRC to not only produce strong research, but to alter the way society perceives data, modeling, and prediction by engaging in joint activities. Hope you will enjoy this issue of the newsletter, where you will find out more about these exciting results.

DAN HENNINGSON
SeRC DIRECTOR

The last annual meeting of SeRC was focused on Big Data and e-Science in Medical Science and attracted 300 participants at Aula Magna, Karolinska Institutet. At the upper left the ERC-president Jean-Pierre Bourguignon (right) is discussing with Carl Johan Sundberg, KI.

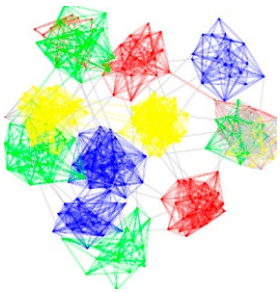
SeSE courses

The Swedish Graduate School in e-Science (SeSE) provides courses in the field of e-Science for PhD-students within Swedish academia. For more information see the web page http://sese.nu.

Scientific highlights

Graph Partitioning for Social Networks and Classification Systems

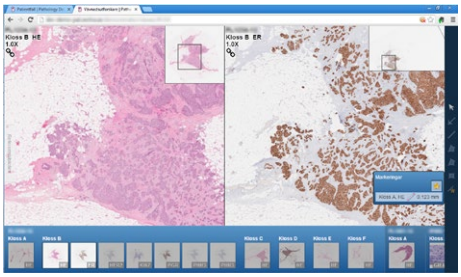
Balanced graph partitioning is a well-known NP-complete problem with a wide range of applications. SeRC researchers from the Distributed and Parallel techniques community have here developed a fully distributed algorithm, which uses local search and simulated annealing techniques. The method, which was awarded with best paper in the IEEE International Conference on Self-Adaptive and



Self-Organizing Systems, 2013, can be easily adapted to any distributed graph-processing system from data centers to fully distributed networks.

Vinnova Framework Grant: Digital Pathology

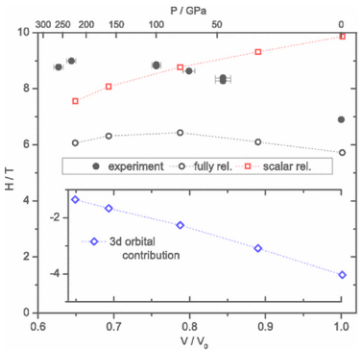
The motivation for this project within the Visualization community is that there is an urgent need for substantially increased efficiency in parallel with continued improvements in quality of care within pathology. Digitisation of histology images is one of few major opportunities to achieve this. The project design includes novel workflows and adapted IT architecture, as well as a prioritized requirement set for corresponding IT tools. The goal for the solutions developed in



the project is to achieve shorter turn-around times in pathology, higher diagnostic precision, more cost-efficient resource utilisation and improved medical education.

Magnetic properties of Nickel at ultrahigh pressure

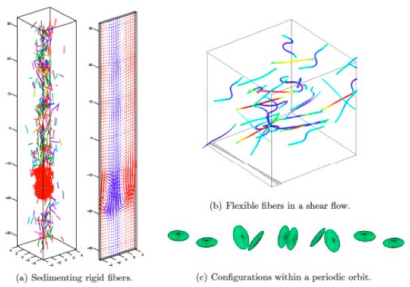
The SeRC Electronic Structure Community has studied the magnetic and elastic properties of Nickel (Ni) at very high pressure, both through experiments and by theoretical electronic structure calculations. Experimentally, it is observed from so called hyperfine splitting that Ni is ferromagnetic up to 260 GPa, the highest pressure where magnetism in any material has been observed so far. At the same time Electronic structure calculations reveal that the pressure evolution of



the hyperfine field, which features a maximum in the range of 100 to 225 GPa, arises from relativistic effect.

Spectrally accurate fast Ewald summation

In molecular dynamic simulations the evaluation of forces resulting from electrostatic interactions requires fast algorithms. Even so, it is often a bottleneck in simulations. A new highly accurate method for this has been developed. The new method has initiated a SeRC project in collaboration between the Numerical Analysis community and the Molecular simulation community



in which the method is implemented in Gromacs and compared to existing state-of-the-art methods.

EC-Earth climate simulations ar contribution to CMIP5 and IPC

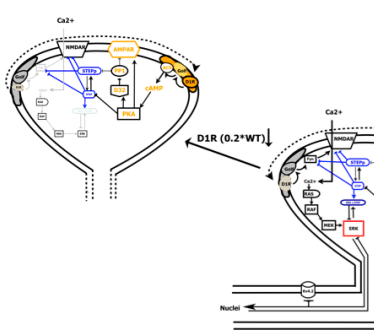
Members of the SeRC Climate Community have performed a large ensemble of historical and future climate simulations using the EC-Earth model as part of the Coupled Model Intercomparison Project Stage 5 (CMIP5), coordinated by the World Climate Research Programme. The model output is stored and made publicly available through the Earth System Grid, a distributed data storage system. The Community has collaborated with the National Supercomputing Centre (NSC) in Linköping to set up a node of the Earth System Grid. The Community has also been

GROMACS: The world's fastest software for Molecular Dynamics on CPUs & GPUs

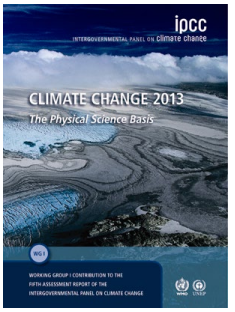
The increase in computing power has increasingly allowed biomolecular experiments to be replaced by simulations. However, designing software that leverages the full power of modern supercomputers is becoming extremely challenging. The GROMACS molecular simulation package is developed and maintained by SeRC researchers, and a great example of the interactions between applications and core e-Science research. SeRC-funded research has increased the parallel scaling fourfold and enabled GPU acceleration that together achieve performance improvements of more

Compartmentalization explains Basal Ganglia neurons of the br

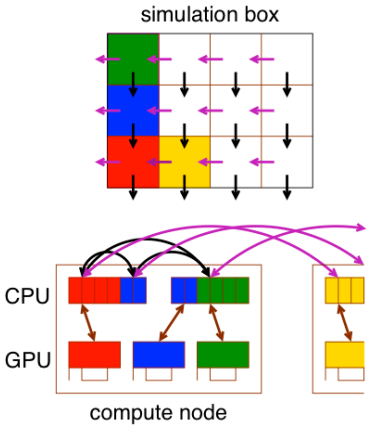
The SeRC Complex Diseases Community has, in collaboration with the Human Brain Project, by integrating data from different sources developed a large computational model of Dopamin signaling related to reinforcement learning in the brain. The model provides an explanation for previously



nd C AR5



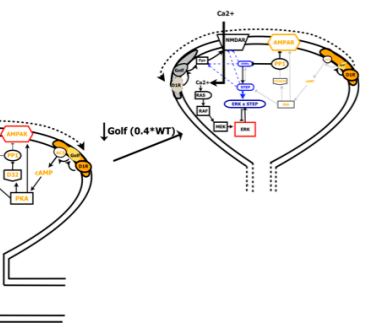
very active in the scientific analysis and interpretation of the CMIP5 climate simulations. This work has fed into the Fifth Assessment Report (AR5) of the Intergovernmental Panel on Climate Change (IPCC).



than an order of magnitude. GROMACS has become one of the most widely used biomolecular simulation codes in the world, with thousands of resulting citations and hundreds of high-impact applications.

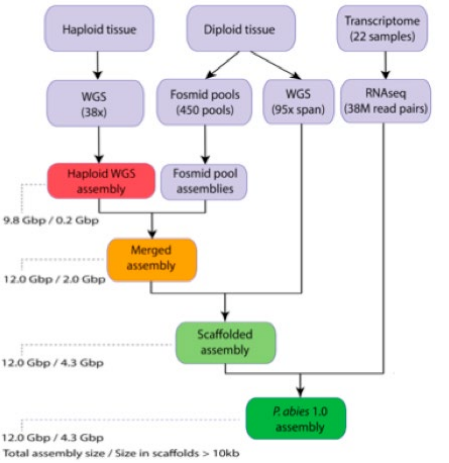
s signaling in rain

unexplained and seemingly inconsistent experimental observations. Through segregation of signaling modules into different subcompartments of the cell, the different data patterns can be reproduced, and this conceives predictions that can be tested experimentally.



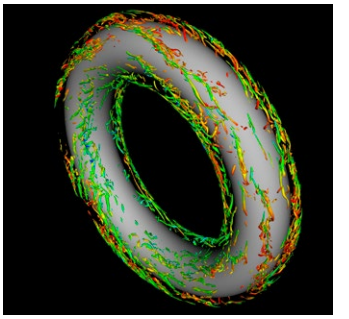
Genome assembly: challenges in the spruce genome project

Conifer genomes are very large; seven times the size of the human genome, something that made the Norway spruce genome project uncertain from the start. It was found that most software for assembling and analysing genomes could not handle the large and complex datasets that the project generated. These problems were met by a combination of experimental and improving computational techniques to which SeRC researchers from the Bioinformatics community have contributed in collaboration with SciLifeLab, and published in Nature 2013.



Turbulence in a Bent Pipe

The FLOW community has been able to simulate particles and turbulence in a bent pipe; all the data was calculated at PDC (KTH Stockholm) using a few thousand cores running the Nek5000 code, and the visualisations were also produced at PDC using VisIt. The figure highlights the action of wall turbulence in the pipe and it becomes clear that e.g. the shear and heat fluctuations on the pipe surface might be very large and lead to "hot spots" and thermal fatigue in, for example, heat-exchanger applications.



In the present simulations, they were able to include for the first time millions of microparticles in such complex geometries.

Beskow: KTH's new supercomputer

Computational research in Sweden is receiving a superb boost in the form of a next-generation Cray XC40 supercomputer that will be available via the Swedish National Infrastructure for Computing (SNIC). The machine, named 'Beskow' is currently being installed at the PDC Center for High Performance Computing at KTH. You can see the stages of the installation as they progress at https://www.pdc.kth.se/resources/computers/beskow/installation-at-pdc

The new Cray XC40 will take centre stage with a peak performance close to 2 petaflops, making it over six times faster than PDC's current flagship system, Lindgren. It is equipped with 53,632 state-of-the-art Intel Haswell cores, and will be the most powerful academic supercomputer system in the Nordic countries.

The system is expected to be in full production on the 1st of January 2015. The new Cray will be an important resource for researchers who run complex simulations in areas such as climate modelling, fluid dynamics, neuroscience, plasma physics, materials science and molecular simulation. SeRC researchers who would like access to the system should apply to SNIC for a time allocation (or, in the case of students, have their supervisor apply for them). For information on applying to SNIC see http://www.snic.vr.se/apply-for-resources.

SeRC Flagship programs

STHLM3 - SeRC e-Science tools evaluate new population-based prostate cancer screening tests

PSA tests are often false positive – is it possible to improve hit rates?

The prostate-specific antigen (PSA) test has a high rate of false positive results leading to unnecessary treatment with life-long complications such as impotence or incontinence. Early results from the Cancer Risk Prediction Center (CRisP) led the Stockholm County Council to fund STHLM3 to collect orders of magnitude more data; the trial recruits 50,000 healthy men aged 50-69 years to assess the test characteristics of a panel of other biomarkers and calculate cost-effectiveness. However, it quickly became a challenge how to handle all data, how to perform image analysis, and in particular how to estimate effects of hypothetical screening scenarios. This led to SeRC establishing a flagship program for "e-Science for Cancer Prevention and Control" (http://www.escience4cancer.net/) to develop tools for this type of research, in particular STHLM3.

SeRC has developed machine learning & simulations to predict screening

The group identified candidate markers and used machine learning to develop the prediction algorithm at the heart of STHLM3. The SeRC team provided input to the design of the trial, including the selection of the paired design and re-screening protocols. We also developed a "microsimulation" framework to compare screening scenarios. This involves the simulation of many individuals, including their cancer history, and screening, on hundreds of cores.
This work established e-Science as a core part of cancer research at KI, with SeRC researchers participating in many different projects.

Unifying clinical medicine, preclinical research, informatics, computer science and education

The e-Science team includes epidemiologists, bioinformaticians, image analysts and computer scientists working on cancer screening. STHLM3 is an even broader collaboration that also involves the County Council, clinicians (oncologists, urologists, pathologists), the biomedical industry, biobank facilities, and laboratories.

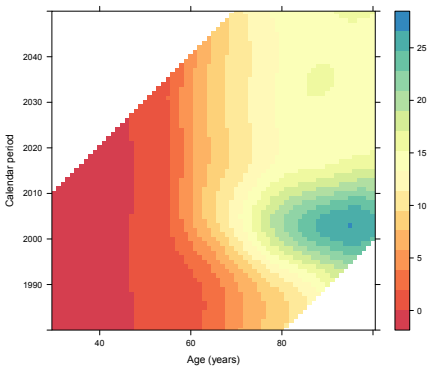
A SeRC student is the first KI PhD to have e-Science in his thesis title and SeRC members are working with colleagues from other universities to extend a course on simulation methods for population health, given for the first time in 2015.

SeRC & STHLM3 is having direct impact on health care and medical industry

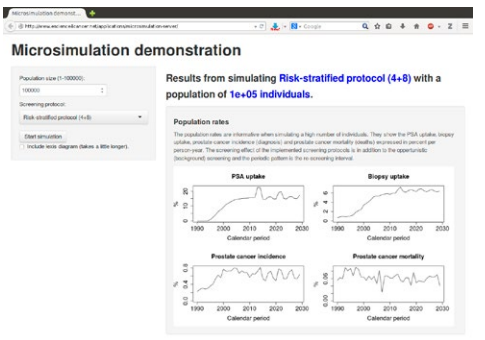
The STHLM3 trial, in combination with e-Science and a unique set of Swedish data resources, will ascertain whether Stockholm County Council should move to organized prostate cancer screening. For the selected biomarkers, we had an industrial partner (Thermo Fisher Scientific) develop a custom chip, and SeRC researchers developed the algorithm and quality assurance methodology. The research has a strong operational focus: how can we change clinical practice to reduce costs from high levels of prostate biopsies, while reducing the possible harms from over-diagnosis and maintaining the mortality benefit from screening?

Using e-Science to handle complex clinical trials might change international practice

STHLM3 has broad interest in the international scientific community. If cost-effective, the study will change international clinical practice. Tentative results from the pilot study suggest that the biomarker panel will reduce the number of prostate biopsies by 20% and will be cost-effective. The integration of e-Science in complex clinical trial design has already had large local impact, and the medical e-Science component is developing into an international strength at KI.



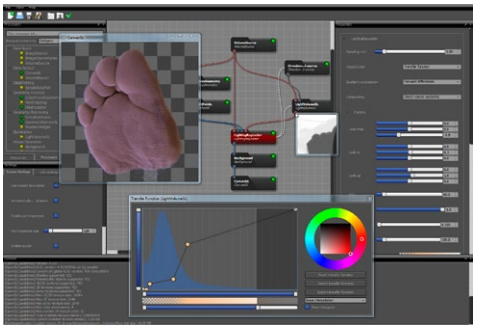
Prostate cancer incidence per 100,000 for Stockholm, assuming continued opportunistic PSA testing. Note how incidence rose following introduction of PSA testing in 1995 and is predicted to decline at older ages below 1990 rates.



Screen-capture of the web-based microsimulation user interface for the the prostate cancer model for a risk-stratified screening protocol, where men at low risk are re-screene every 8 years and medium risk every 4 years.

Collaboration through Visualization

A collaboration tool for SeRC researchers has been developed within the SeRC visualization flagship program through an extension of the visualization software Inviwo. To make Inwivo applicable within SeRC, demands of different disciplines have been taken into account and appropriate Inviwo modules developed. In some cases, also the core functionality has been extended to better serve the needs of the collaboration partners. Successful collaborations using Inviwo includes the area of material sciences, solar cell design, molecular dynamic simulation and medical visualization. An interactive Bader analysis application, for instance, enables material science researchers, to interactively inspect the 3D structures of crystals in a visual manner. Advanced molecular rendering techniques enable solar cell designers and molecular dynamics researcher to better understand their simulation data, whereby even large data sets can be visualized. More information can be found at http://www.e-science.se/flagship/collaborative-visualization.



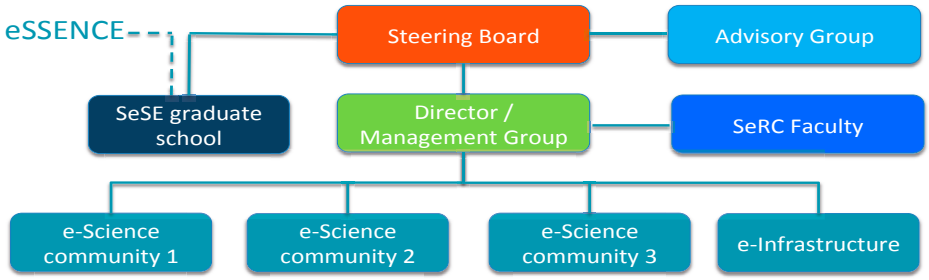
SeRC Exascale Simulation Software Initiative

New supercomputers like Beskow are amazing resources, but pose tremendous challenges to software – to utilize the power of the new Cray in Stockholm, computer programs need to scale to 100,000, and in the near future a million, processes.

The SeRC flagship program SESSI deals with Exascale simulation challenges, many of which are common across different application areas. SESSI is a collaboration between three SeRC communities (Molecular Simulations, FLOW, Distributed and Parallel Techniques) and the CRESTA EU project. SESSI has already lead to developments and cross-fertilization between the fluid dynamics software NEK5000, and the molecular simulation code GROMACS. More information can be found at http://www.e-science.se/flagship/sessi.

SeRC Organization and Activities

Morten Dæhlen, University of Oslo, new external chairman of the SeRC research center board of directors.



Vision: "Through e-Science enable world leading research within strategic areas."

Universities: Collaboration between Kungliga Tekniska högskolan (KTH), Stockholms universitet (SU), Karolinska institutet (KI) and Linköpings universitet (LiU).

Steering Board: SeRC is now a formal center, hosted at KTH with five members of the Board; Morten Dæhlen (Chairman), University of Oslo; Mattias Sillén, SAAB group; Arne Johansson, KTH; Gunilla Svensson, SU; Anders Ynnerman (Deputy Chairman), LiU, Juni Palmgren,KI

Advisory Group: Including international representatives and members from both academia and industry to ensure an industrial perspective on our research and to facilitate collaboration with society.

Management Group: Is led by the Director, Dan Henningson, with help from Co-director Erik Lindahl, and Coordinator Olivia Eriksson, and consists of people from the Faculty and Communities.

SeRC faculty:

- Consists of all community coordinators and senior researchers with substantial funding from SeRC.
- Main goal to facilitate interdisciplinary exchange between applied and core e-Science communities, and to provide SeRC with an inter-community-network of e-Science scientists. The faculty is advising the director and management on scientific issues.

e-Science Communities:

- 10 research communities in which we promote the collaboration between e-Science applications, core e-Science and application experts at NSC and PDC.
- Each community is led by a coordinator, funded from SeRC, who initiate and manage the SeRC e-Science projects, is responsible for a range of community activities, as well as liaising with other national and international communities.

Infrastructure:

- **Supercomputer centra:** Center for High Performance Computing (PDC) , KTH, National Supercomputer Centre (NSC), LiU
- **Application Experts:** employed at the supercomputer centra, but working close with the e-Science communities
- **Visualization centra:** Visualization Center C, Norrköping, Visualisation studio at KTH (VIC)

SeSE graduate school:

- SeRC has, together with eSSENCE, a graduate school in e-Science, the national Swedish e-Science Education graduate school (SeSE)

Industry and Society:

- SeRC has an industry-coordinator partly employed by SeRC, a large number of collaborative projects with industry (http://www.e-science.se/industry) and half of our Advisory-group comes from industry.
- SeRC engages broadly with society and our research has direct impact, e.g. through our Climate and Cancer research.

Regular activities:

- Annual meetings for all SeRC members, about 100 participants every year
- Arranging conferences, e.g. '7th IEEE International Conference on e-Science' (Dec 2011) and 'EASC2014: Solving Software Challenges for Exascale' (April 2014)
- Arranging seminars, e.g. a seminar with the 2013 Chemistry Nobel laureates Martin Karplus discussing creativity.
- Community meetings and seminars, e.g. kick-offs, lunch-meetings, seminar series.
- SeRC faculty has 1–2 larger meetings each year, often together with team-building organization consultants. The application experts and steering board has also taken part in these meetings.
- Management-group meetings (monthly) as well as steering-board meetings (3–6 times per year). Follow-up meetings, for internal revision, with communities and the management.
- A large number of courses within SeSE
- SeRC members regularly make presentations at schools and museums, are interviewed in media about their research and contribute to the societal discussion e.g. through the intergovernmental panel on climate change (IPCC)

Website: http://www.e-science.se

Annual Meeting 2015

The sixth annual meeting of SeRC will take place 15th –16th of June, 2015. Location to be announced.

Printed by LiU-Tryck, Linköping

Swedish e-Science Research Centre,
SE-100 44, Stockholm, +46 8 790 7570, info@e-science.se
Editor: Olivia Eriksson For a paper version or PDF-file send an e-mail to info@e-science.se.