SeRC

Swedish e-Science Research Centre

Five-year progress
Organisation
Future plans

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THE CONCEPT OF e-SCIENCE

In its most basic form, the concept of e-Science is simply the notion of using digital information and the processing of this information to gain new scientific insights.

SeRC LEADERSHIP

Dan Henningson Director, KTH
Erik Lindahl Co-director, SU
Olivia Eriksson Coordinator, KTH
Morten Daelen Chairman of the board, University of Oslo
Anders Ynnerman Vice chairman of the board, LiU
Juni Palmgren University representative, KI
Gunilla Svensson University representative, SU
info@e-science.se, www.e-science.se

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Editing, form, layout, illustrations: Gunnar Linn, Linnkonsult www.linnkonsult.se
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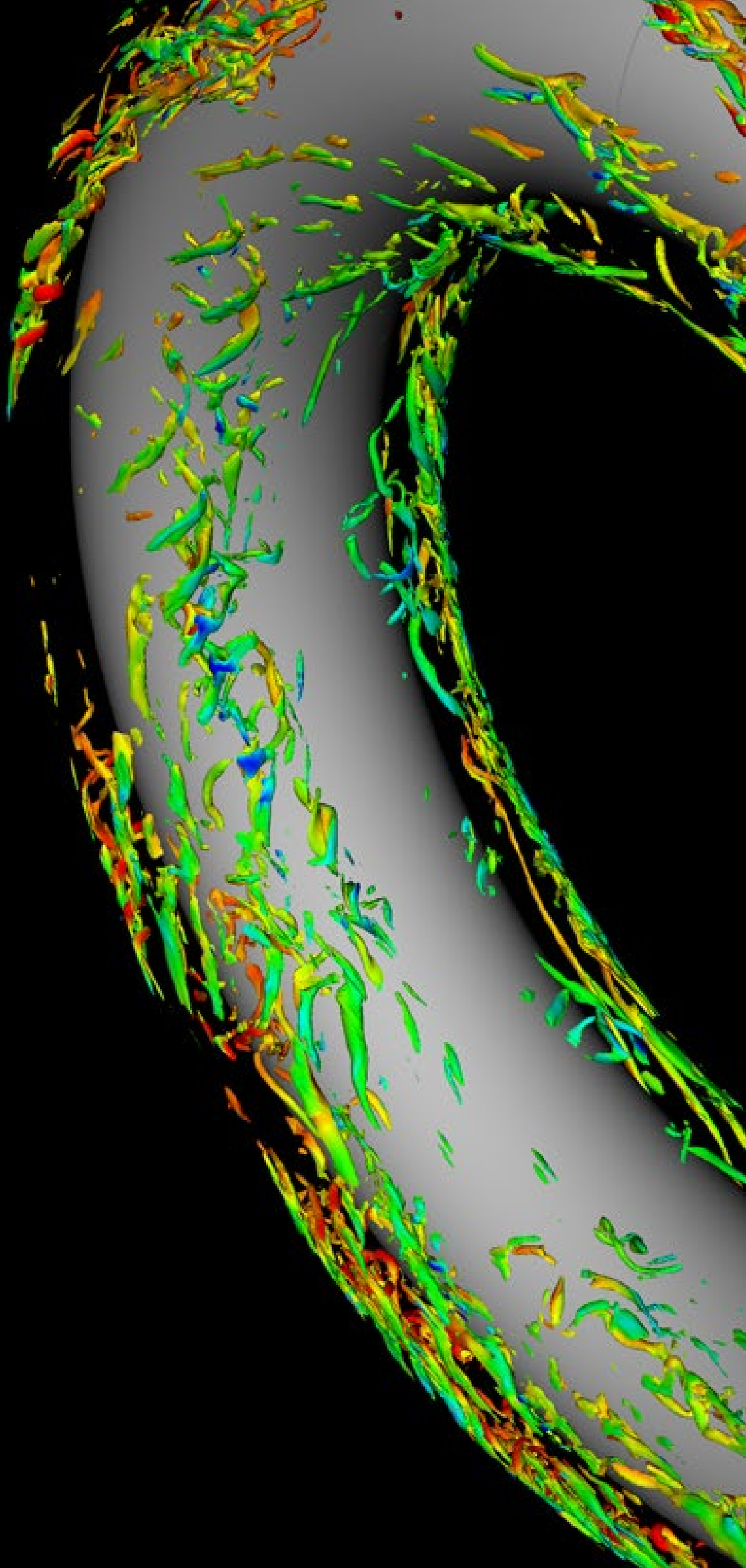
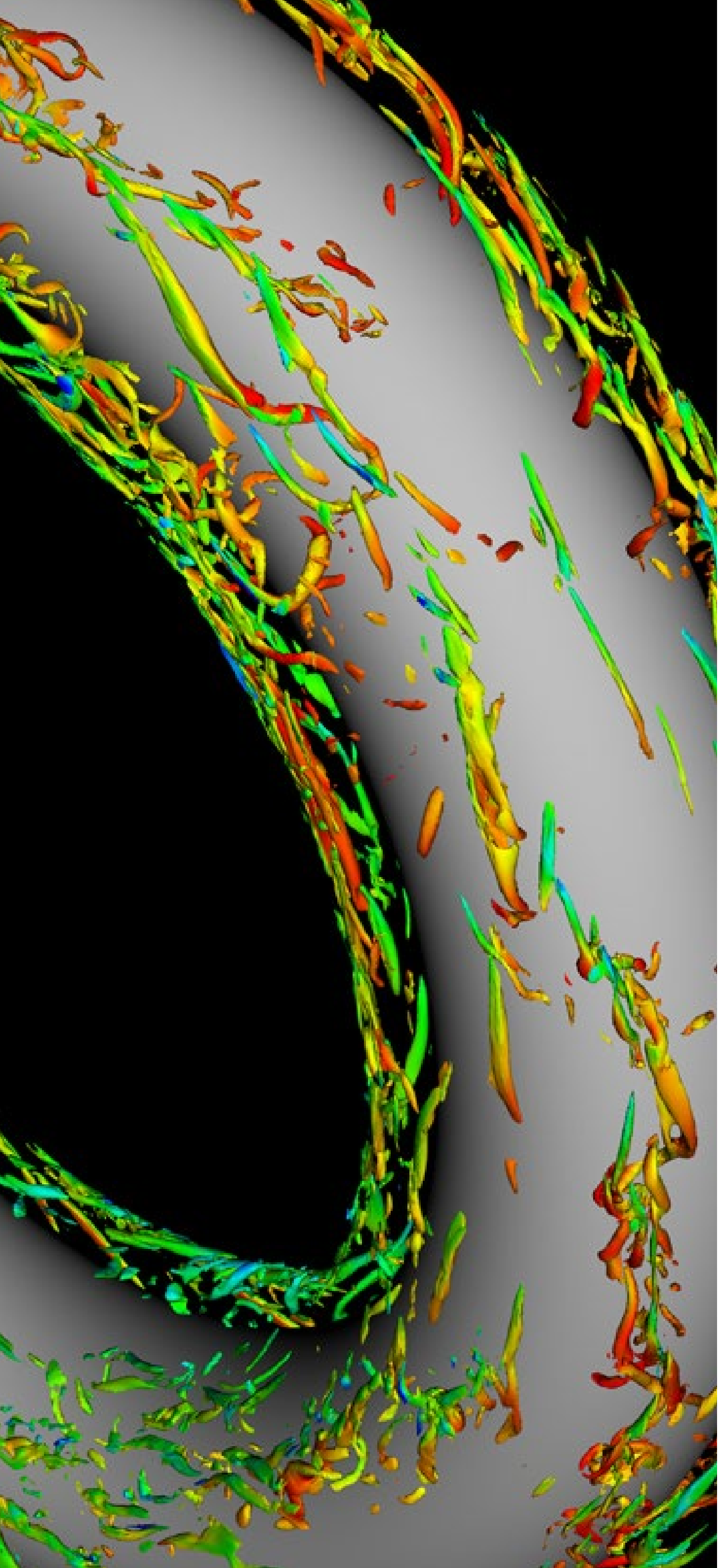




Welcome to SeRC!

SeRC – A STRATEGIC RESEARCH CENTRE

SeRC is a strategic research centre within the strategic research area (SRA) of e-Science, funded by the Swedish government Strategic Research Area Initiative and based on a collaboration between four universities: Kungliga Tekniska högskolan (KTH), Stockholms universitet (SU), Karolinska institutet (KI) and Linköpings universitet (LiU). It was founded in 2010 resulting from the Swedish Government Bill on Research Policy. In this bill, a total of 24 different strategic research areas were defined, of which e-Science is one.

The mission statement of SeRC is to develop state-of-the-art e-Science tools and provide an e-infrastructure support to existing and emerging e-Science communities to achieve scientific breakthroughs in Sweden.

FUTURE ACTIVITIES

Multidisciplinary collaboration programmes

SeRC will develop multidisciplinary collaboration programmes in strategic areas with high potential gain, by consolidating the SeRC efforts into larger constellations. Read more on page 18.

Scientific computing lab

Following international examples, for instance from NCSA at UIUC, SeRC will prototype a scientific computing lab, where researchers from applications, methods, and infrastructure can collaborate, forming the ”human e-Cloud”. Read more on page 18.

Data-driven science

SeRC will help transfer knowledge on the use of methods and tools from data science to enable new research methodologies in SeRC communities and for other Swedish e-Science researchers. Read more on page 19.

1. e-Science and SeRC

Science is currently being redefined by the use of computers. New scientific insights are gained by using and processing digital information. SeRC pushes the limit of what can be achieved.

WHAT IS e-SCIENCE?

We are right in the middle of a revolution where computers are redefining science as we know it. While the trend started in the natural and engineering sciences, it has evolved to become a pervasive component of virtually all scientific fields: modern aeroplane design depends more on computational fluid dynamics than wind tunnels, bioinformatics has turned biology into a quantitative subject, and we are seeing entirely new data-driven science, for instance in medicine.

Many of the challenges faced are similar: all these research directions rely on access to large computational resources, ability to work with and archive huge amounts of data, new algorithms both for computation and large-scale data analysis, and not least providing career paths for the highly skilled computational staff we recruit.

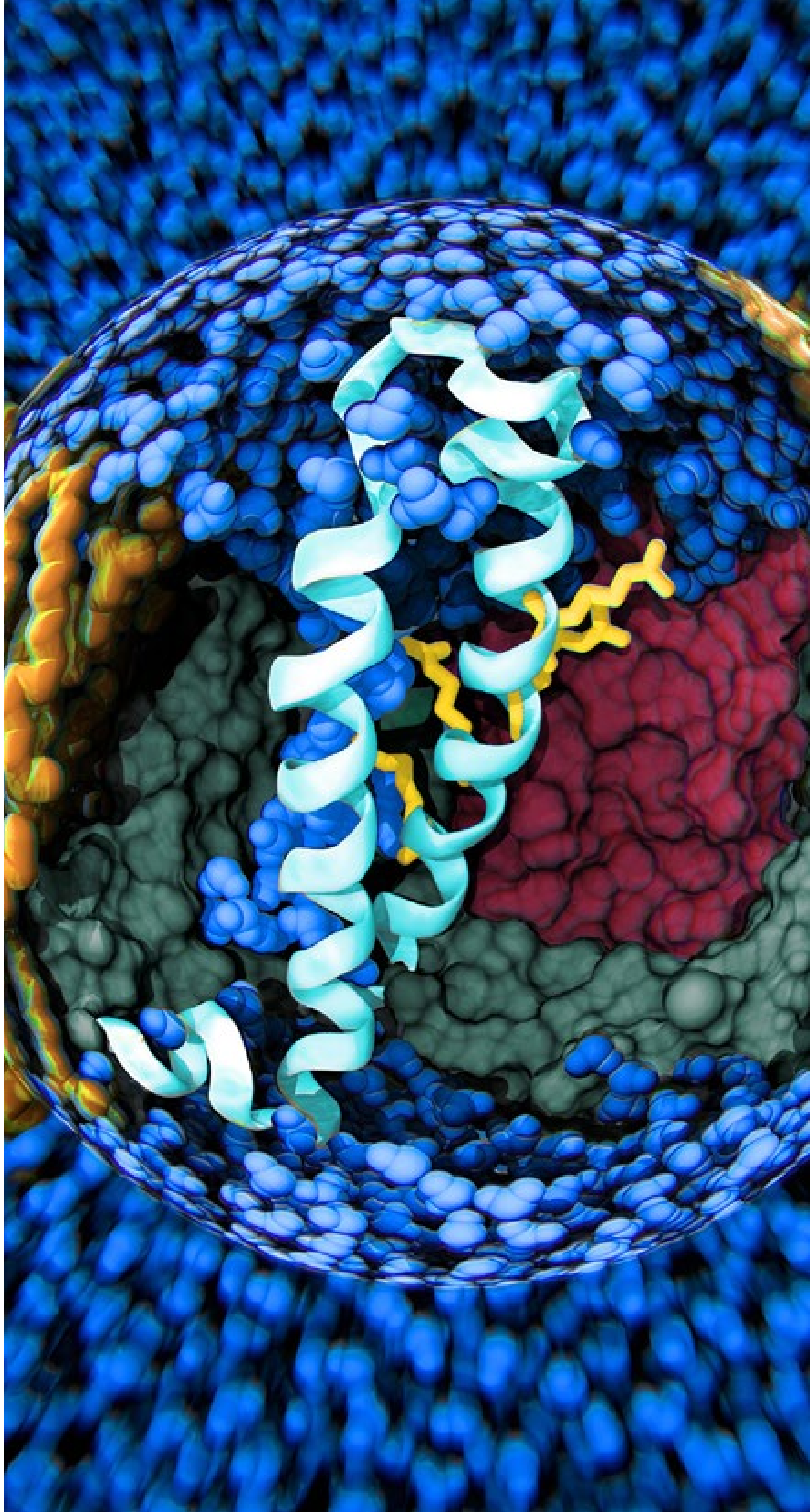
In its most basic form, the concept of e-Science is simply the notion of using digital information and the processing of this information to gain new scientific insights. This means that much of what we could call e-Science can be conducted using standard solutions both in terms of hardware and software.

> Much of what we could call e-Science can be conducted using standard solutions both in terms of hardware and software."

SeRC AND OUR MISSION

SeRC's scope is to address problems that go beyond standard solutions and are in need of access to state-of-the-art e-infrastructure as well as demanding new e-Science methodology and technology, thereby pushing the development of new e-Science tools. In this way SeRC paves the path for new high-end e-Science that will eventually mature and benefit not only the groups involved in SeRC but also the whole academic base of e-Science users.

> SeRC's scope is to address problems that go beyond standard solutions, thereby pushing the development of new e-Science tools."



OUR THREE-PILLAR MODEL

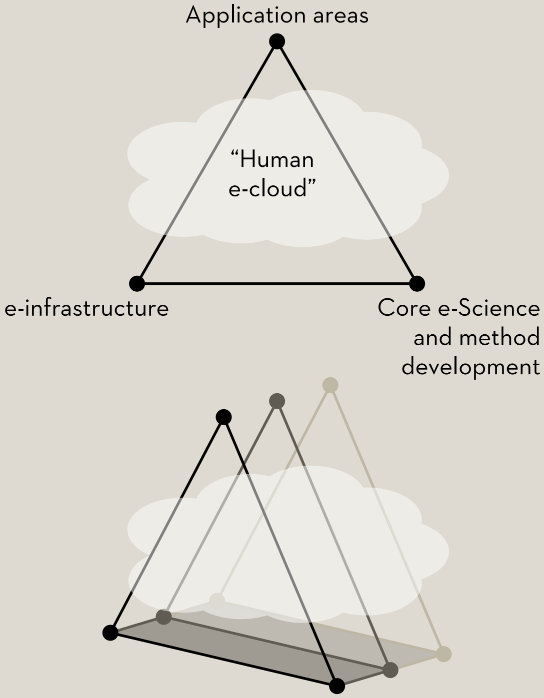


Figure 1. Our three pillars are ***application areas, e-infrastructure,*** *and* ***core e-Science and method development.*** *The two bottom pillars are mutual for different application areas.*

The work in SeRC relies on three pillars of existing excellence in application areas, method development, and e-infrastructure, connected through a "human e-cloud".

Pillar 1 – application areas: It's a central goal for SeRC to have direct impact in *application areas* of strategic relevance for our partner universities, and conversely we want to focus on topics where SeRC has world-leading research groups. In particular, this includes fields such as computational fluid dynamics, materials science, bioinformatics, molecular simulation, climate modeling, and cancer epidemiology and screening (see our success stories in chapter 2).

Pillar 2 – e-infrastructure: We want to facilitate the development of a world-class *computational infrastructure* at PDC, NSC, and the visualisation centres. This includes competitive hardware investments in collaboration with The Swedish National Infrastructure for Computing (SNIC), but it's equally important to recruit advanced infrastructure experts to build a culture of international expertise, excellence, and infrastructure collaborations targeting development of key codes rather than merely providing user support.

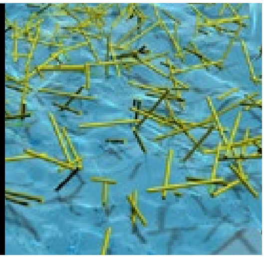
Pillar 3 – core e-Science and method development: An integral part of SeRC is leading-edge research in core *e-Science and method development,* for instance in fields such as numerical analysis, visualisation, parallelisation, acceleration, and data engineering. The core research groups contribute both with the latest research results on e-Science tools as well as a broad competence base in e-Science tool usage and methodology.

The "human e-cloud": For SeRC, the central challenge is to get these three pillars to strengthen and support each other through collaborations. Infrastructure and core e-Science do not exist in vacuum, but should engage directly in important application research, and at the same time SeRC only supports application areas where we see an opportunity to translate advances in fundamental e-Science into research impact.

Our primary tool to achieve this is the recruitment of e-Science experts that work cross-disciplinary between these areas, what we have designated as a *"human e-cloud".* These experts combine a deep knowledge of the application area with expertise either in method development or large-scale computational infrastructure. By integrating these e-Science experts into the research environments, there will also be new opportunities for close collaborations between experts facing similar challenges (for instance in parallelisation, data management or method development) in different application areas.

SeRC'S MISSION STATEMENT

SeRC's mission is "to develop state-of-the-art e-Science tools and provide an e-infrastructure support to existing and emerging e-Science communities to achieve scientific breakthroughs in Sweden".



OUR THREE-PILLAR MODEL

To address this scope, SeRC uses a three-pillar model (see fact box above) in which existing excellence in *application areas, core e-Science and method development*, and *computational infrastructure* are combined to enable research teams to work closely together. In particular, this is done through collaborations and e-Science experts active in at least two of these pillars.

Long-term, our vision is to better address challenges that are common to different application areas, and to develop a *"human e-cloud"*.

e-SCIENCE INFRASTRUCTURE

Two supercomputer centres: PDC Center for High Performance Computing at KTH (PDC) and National Supercomputing Centre at LiU (NSC) – both part of the Swedish National Infrastructure for Computing (SNIC);

Two visualisation centres: Visualization Center C (VC), Norrköping and the Visualisation Studio at KTH (VIC);

A number of e-Science experts who are employed at the supercomputer centres, but work closely with the research communities.

ORGANISATION

SeRC consists of ten *research communities,* within which the e-Science research take place, together with the *e-Science infrastructure* (see info box). Some of the communities focus on core e-Science methodology, like numerical analysis, parallel software and data engineering and visualisation, whereas other focus on some area of application of this methodology, like

> By any measure, SeRC has been a great success scientifically."

bioinformatics, neuroinformatics, cancer epidemiology and screening, molecular simulations, electronic structure, computational fluid dynamics, or climate research.

SeRC co-finances about 30 projects and 15 faculty positions, including a number of larger *multidisciplinary collaboration programmes* that were initiated in order to increase collaboration between application, core and infrastructure (see figure 1 on page 5).

More info about the SeRC organisation can be found at **www.e-science.se/org**.

FOCUS AND IMPACT

SeRC's collaborating partners – KTH Royal Institute of Technology, Stockholm University, Karolinska Institutet, and Linköping University – host strong research fields, and SeRC has been instrumental both in helping the universities to focus on their key strengths and forming joint research communities – but also to de-emphasise areas where another partner had a better position.

This has led to significantly increased collaborations, a large number of high impact publications, and several new cross-disciplinary research projects and infrastructure grants – which did not exist prior to SeRC. By any measure, SeRC has been a great success scientifically, and we have had the privilege of a very engaged scientific advisory committee.

SeRC will remain a dynamic organisation that pushes the frontiers of research. One current example of this is to find ways to combine data-driven research methods with the strong Swedish tradition in engineering and simulation-driven science, where several leading SeRC research teams have now formulated exciting new collaborations that we hope will have large impact in the next few years.

2. The first five years

Founded in 2010, SeRC was granted five years of initial funding. This is what we achieved during this time.

SeRC FACULTY

During 2010–2014, SeRC has built an organisation that enables world-leading research within areas that are strategically important for Sweden, in particular through multidisciplinary collaborative efforts at different levels in the e-Science landscape.

> SeRC has built an organisation that enables world-leading research within areas that are strategically important for Sweden.”

Since the start, we have recruited a substantial number of highly skilled assistant professors. In addition, we have selected a number of e-Science investigators who either were recently hired, or recently joined SeRC with other funding. Together, these researchers form the *SeRC faculty.*

The main goal of the faculty is to facilitate interdisciplinary exchange between e-Science communities in application areas and core e-Science and method development (the top and lower-right pillars in figure 1 on page 5), and to provide SeRC with an inter-community network of e-Science scientists. For the first time, SeRC now enables long-term funding for leading scientific software development in Sweden.

The success of the SeRC project is reflected by the excellent grades that SeRC received in the evaluation of the government investments in strategic research areas (see fact box on page 8).

COLLABORATION

SeRC hosts a large number of outstanding scientists who are pushing the state of the art in applications and method development, with several high-impact results. However, SeRC’s mission is to go a step beyond merely providing funding and rather build a scientific environment that promotes disciplinary excellence through multi-disciplinary collaboration.

SeRC makes it possible to initiate new, ambitious, and risky collaborative projects that have the potential to redefine research fields. In particular, the centre has catalysed the formation of several strong environments that work on the application, method-development and infrastructure aspects of computational research. These multidisciplinary collaborative projects for instance make it possible to engage computational experts in long-term development efforts that previously have been very difficult to fund.

The new initiatives have had tremendous scientific impact: One of the SeRC software

FROM THE SRA EVALUATION
The Swedish Research Council has led an evaluation of the SRA initiative that was presented for the government in May 2015. An expert panel carried out the evaluation with help from external reviewers. Below are some quotations from the report.

- "The expert panel concludes that the investment in Strategic Research Areas has been an excellent and original initiative from the Swedish Government. According to them, one of the main strengths of the strategic research investment has been its long-term focus. This has made it possible to combine risk-taking and high ambitions in research and in the recruitment of new personnel – both junior researchers and internationally leading researchers – as well as developing new research areas."
- "In e-Science, a strong national network was founded between KTH, Linköping and Stockholm Universities and Karolinska Institute."
- "KTH has ... excellent ... SRAs". (One of the two acknowledged was SeRC.)

FROM THE SeRC EVALUATION
Performance: Excellent/good
Strategy: Excellent/good
Added value: Excellent
"The research in this group appears to be internationally competitive. The SRA funding has enabled development of infrastructure and collaboration. Their strategy has been to identify the best groups from a development and exploitation perspective and connect them across the 4 participating universities. They have promoted the use of e-Science in these communities and systematically bridged the gap between tool developers and the actual users. They feel that SRA funding has increased their capacity to work with industry and they have a long list of industrial collaborators."

"A national graduate school has been developed using SRA support in order to develop existing initiatives. Their aim is to make this a Nordic school. Within this SRA, the Advisory group appears to have been particularly strategic and has encouraged the community to develop 'flagship' projects not included in the original proposal."

LARGE-SCALE COMPUTING
In January 2015, the SeRC infrastructure got a significant boost with the inauguration of Beskow at PDC – a 2-petaflop Cray XC40 system, more powerful than all other SNIC systems together. With Beskow, SeRC researchers for the first time have a world-class petascale system at their disposal, much needed for their research and also as a stepping stone towards the larger European-level infrastructure. Beskow was designed to cater to the needs of SeRC and important SeRC applications were used as benchmarks to guide the selection process.

In autumn 2017, NSC's flagship system, Triolith, will be replaced with another petascale system, ensuring that SeRC researchers and other e-Science researchers in Sweden continue to have access to the latest hardware technologies.

projects became Sweden's single most most cited scientific paper during 2014, teams who did not even know each other prior to SeRC have merged, and the collaborations between infrastructure and researchers have led to a range of new high-profile international research projects being funded, not to mention several prestigeous ERC grants.

However, instead of being content, we will keep raising the bar by continuously evaluating our collaborations with a critical eye to justify the centre's existence. SeRC's goal is not to maintain the status quo, but to promote discoveries and new applications by helping and forcing talented researchers to team up and leave their comfort zones. Collaboration, multidisciplinarity, change, and impact are in the genes of SeRC.

SCIENTIFIC OUTPUT

SeRC has been the driving force behind a strong development in SeRC researchers' publication quality and volume during the period 2010–2014. In particular, the synergies stemming from new interdisciplinary collaborations promoted by SeRC have made a mark on the publication profile. The publication output by SeRC research projects has almost doubled from 2010 to 2014, as the funded projects have started publishing results.

An explicit goal of SeRC was to enhance research quality, and we have a

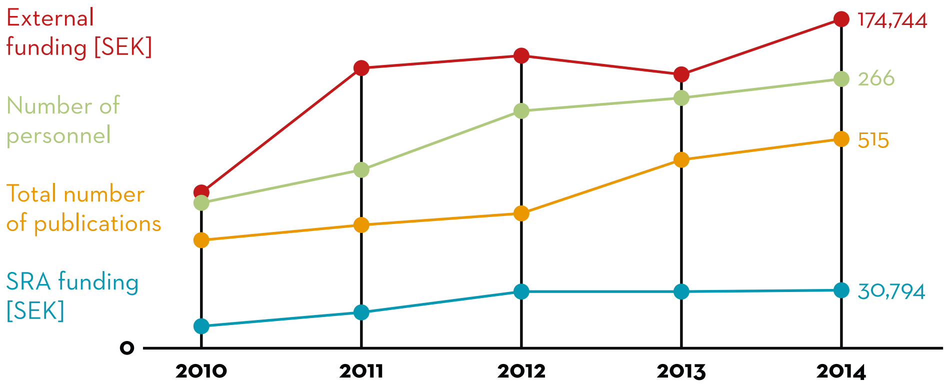


Figure 2. Progress 2010–2014.

number of publications in Nature, Science, and top-ranking journals in each field. Considering that SeRC financing is a small part of the total financing to SeRC researchers (about 17%, 30 MSEK out

> This is a strong indication of the synergy effects of SeRC."

of 175 MSEK for 2013), this is a strong indication of the synergy effects of SeRC. A measure of the impact of the publications is that SeRC researchers have an average field-normalised citation rate of 1.92 during 2010–2014, which is almost double the world average.

COMPUTING RESOURCES

e-Science is critically dependent on efficient large-scale computing and storage resources. Within SeRC, these resources are provided by the leading Swedish high-performance computing centres – PDC and NSC – which offer more than two thirds of the Swedish national compute capacity. A strategic partnership among these has been established. This allows for better coordination and alignment of their services towards the needs of SeRC researchers.

Since 2015, SeRC has access to petascale computing resources (see fact box) throught these centres. But it is noteworthy that PDC and NSC not only provide hardware, they also provide expertise in many application areas in terms of computing experts that work closely with certain scientific domains, including bioinformatics, climate modelling, computational fluid dynamics, materials science, molecular dynamics, and neuroinformatics.

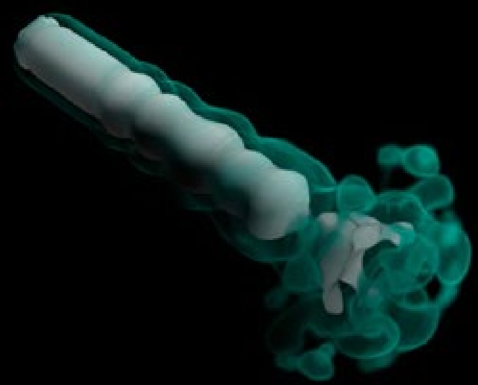
FORMAL RESEARCH CENTRE

In December 2013, to consolidate the organisation, SeRC turned into a research centre with KTH as host, and we recruited an external chair of the board, Professor Morten Dæhlen, Dean of Mathematics and Natural Sciences at the University of Oslo and a prominent international e-Science leader.

More info about the SeRC organisation can be found in the introduction chapter and at **www.e-science.se/org**.

SUCCESS STORIES

Please join us for a brief exhibition of some of the projects that we have been managing at SeRC during our first five years.



SUCCESS STORY: **CLIMATE MODELLING**

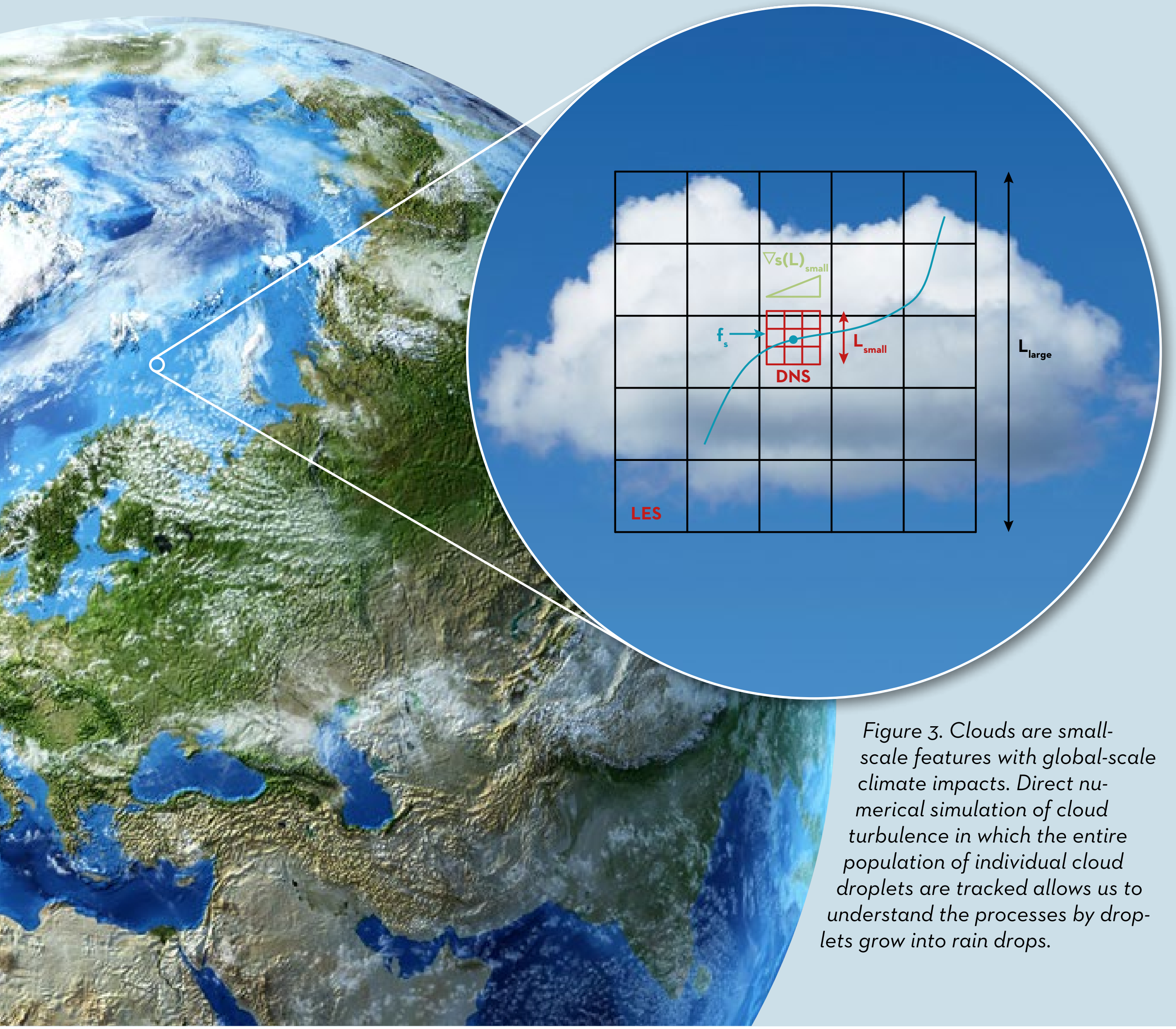


Figure 3. Clouds are small-scale features with global-scale climate impacts. Direct numerical simulation of cloud turbulence in which the entire population of individual cloud droplets are tracked allows us to understand the processes by droplets grow into rain drops.

Climate is a prime example of a “multi-scale” system: important phenomena occur on a spectrum of scales spanning from global circulation (104 km) to cloud-scale processes (1 cm). The SeRC Climate Modelling community has made substantial progress in modeling processes at both ends of the spectrum and understanding their cross-scale interaction.

At the global scale, we have contributed to the development of the EC-Earth global climate model (**www.ec-earth.org**), notably via a SeRC-funded postdoc at SU who developed a simplified, single-column version of the model to understand the impact of local cloud-scale processes on the larger scales. Together with partners at SMHI, we also conducted a large set of global-scale simulations which directly contributed to the International Panel on Climate Change Fifth Assessment Report, released in 2013, which is the key document providing scientific guidance on climate change to policymakers worldwide. The availability of a dedicated climate e-Science expert has been essential in enabling these contributions.

At the small end of the spectrum, we have collaborated with the FLOW community at KTH through another SeRC-funded postdoc to apply direct-numerical-simulation methods originally developed for engineering applications to better understand how cloud turbulence helps produce rain, making an important theoretical breakthrough in this direction published in *Physical Review Letters* 2015.

Read more on **www.e-science.se/climate-modelling**

Main position in our three-pillar model (see page 5)

SUCCESS STORY:
PERSONALISED CANCER SCREENING (ECPC)

E-Science for cancer prevention and control (ecpc.e-science.se) is a SeRC flagship project that focuses on integrating novel findings from bioinformatics and image analyses with the Swedish nationwide registers and cohort studies in the population. eCPC utilises this ensemble of data for modelling the natural history of cancer and personalised cancer screening.

The ultimate goal is to design trials and to evaluate public policy shifts for cancer screening using micro-simulation, creating better ways to screen cancer. Personalised cancer screening is expected to change clinical practice, improve population health and potentially reduce health care costs.

eCPC integrates scientific expertise in computer science, statistics, and mathematics with expertise in molecular medicine and clinical epidemiology for prostate and breast cancer. For prostate cancer, a full-scale personalised prostate-cancer diagnostic pipeline is being created using a combination of genomics, proteomics, and imaging.

An important landmark is the STHLM3 study, which recently reported on a prospective evaluation of the novel *S3M* prediction algorithm as a screening tool. Developed in close collaboration with SeRC researchers, S3M is superior to the currently used PSA test and the Stockholm County Council has planned for a clinical roll-out of S3M during 2016.

Together with a large managed care organisation in the US, a large-scale implementation of S3M is being planned, including the validation of S3M across four ethnic groups.

Read more on www.e-science.se/ecpc

Figure 4. eCPC is developing, implementing, and evaluating methods for using large amounts of biomedical data for risk-stratification in cancer screening and diagnosis.

ecpc

e-Science for Cancer Prevention and Control

Main position in our three-pillar model (see page 5)

SUCCESS STORY:
"VIRTUAL WIND TUNNEL"

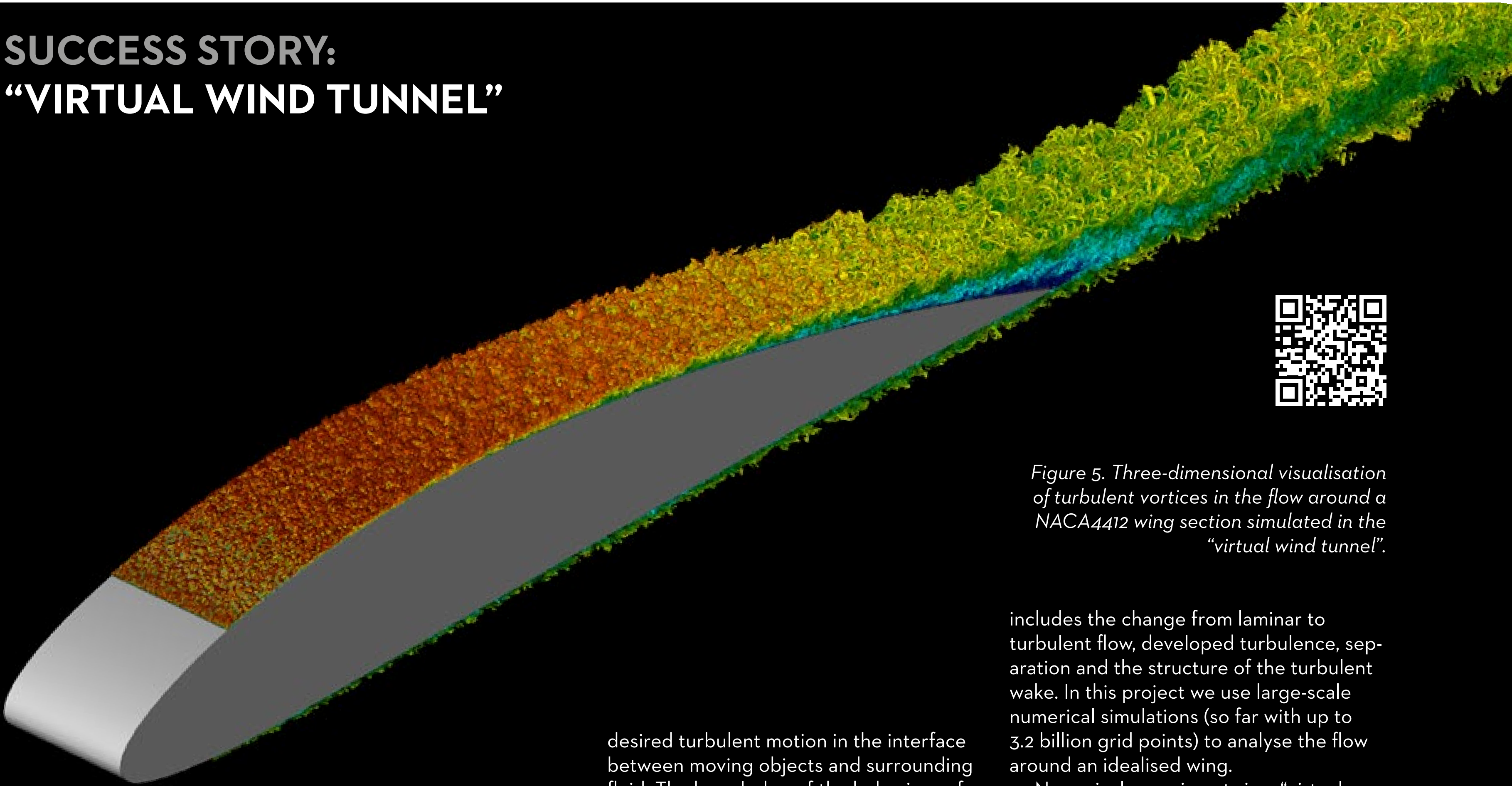


Figure 5. Three-dimensional visualisation of turbulent vortices in the flow around a NACA4412 wing section simulated in the "virtual wind tunnel".

Automotive, aeronautic, and maritime transport of people and goods play important roles in the globalised world, but are also using up about five billion barrels of oil per year. Roughly half of the energy being spent worldwide in such transport activities is dissipated by undesired turbulent motion in the interface between moving objects and surrounding fluid. The knowledge of the behaviour of turbulence close to these surfaces is of paramount importance if optimal design and perhaps drag reduction via flow control is attempted.

Accurate numerical simulations allow the characterisation, with the highest level of detail, of the multiple physical phenomena present in complex flow cases such as around airplane wings. The physics includes the change from laminar to turbulent flow, developed turbulence, separation and the structure of the turbulent wake. In this project we use large-scale numerical simulations (so far with up to 3.2 billion grid points) to analyse the flow around an idealised wing.

Numerical experiments in a "virtual wind tunnel" and the concept of "virtual wind tunnel" aims at replacing, in the future, some real wind-tunnel experiments by corresponding simulations, which will yield a much larger wealth of data relevant for design purposes.

Read more on www.e-science.se/flow

Main position in our three-pillar model (see page 5)

SUCCESS STORY:
GROMACS – MOLECULAR SIMULATION

Molecular simulation has become a cornerstone both in materials and biomolecular research, and it is one example where SeRC has enabled a new type of three-way collaborations between application areas, infrastructure, and method development. The GROMACS code developed at Stockholm University and KTH has grown into one of the world's most widely used molecular-dynamics implementations, with thousands of active users both in academia and industry.

Together with several partners such as NVIDIA, Intel, AMD, Stream-Computing, and IBM, SeRC and the GROMACS team have developed new generations of heterogeneous acceleration and parallelisation algorithms that achieve world-leading simulation performance on all sorts of hardware from embedded graphics processors to supercomputers.

This computational work has been instrumental for several high-impact application works where SeRC researchers have shown phenomena such as how ion channels open, and how membrane proteins bind specific lipids, structures of new transporters, collaborations with the electronic structure community on multiscale QM/MM simulations, and not least explanations of how the outermost layer of our skin forms on the molecular level.

SeRC has also been a very strong driving force to form close and long-term collaborations with the infrastructure efforts at PDC and the Computational Fluid Dynamics team, which has led to new joint programmes on exascale simulation software as well as the BioExcel EU Centre of Excellence for Computational Biomolecular Research in Stockholm.

Read more on www.e-science.se/molecular-simulation

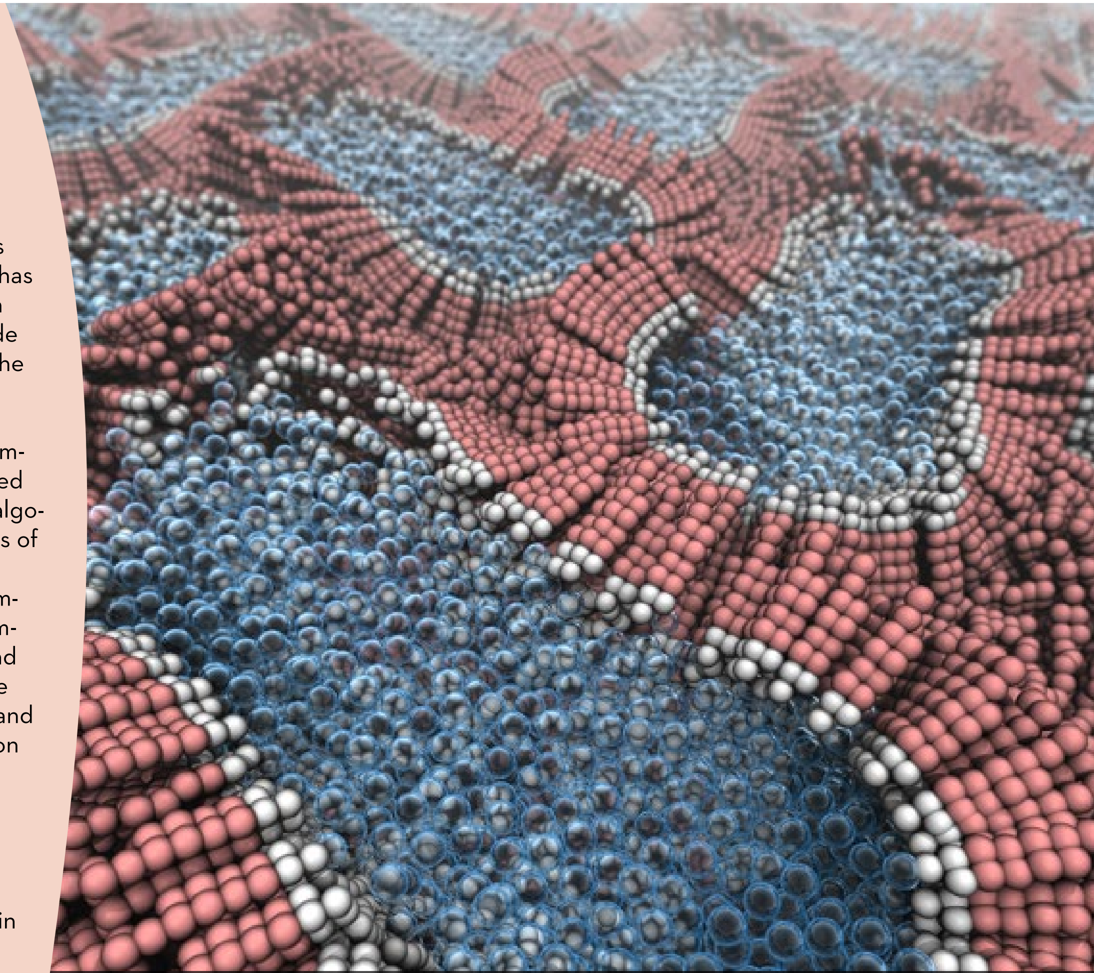


Figure 6. We know surprisingly little of how drugs penerate skin, and it is very hard to design new such drugs since we do not yet understand the molecular organisation of skin. SeRC has used coarse-grained molecular simulations to describe the process where ceramides and other lipids fold into multiple layers forming the stratum corneum outer skin through intermediate cubic phases. By comparing with cryo-electron microscopy images of skin obtained at the Karolinska Hospital it has been possible to validate these models, which are now being used for targeted drug transport design in collaboration with industry.

Main position in our three-pillar model (see page 5)

SUCCESS STORY: VISUALISATION

With the advent of big data resulting from simulation and imaging, visualisation becomes an essential tool for accessing and understanding the generated data. Thus, the SeRC visualisation community serves as a core community within SeRC, whereby the conducted research gives other SeRC researchers the opportunity to analyse their data. As a consequence, traditionally within the visualisation community, the connection to the other communities is central in order to enable a fruitful research output.

A prominent example of this intercommunity work is the long-standing cooperation with the material-science community, in which an interactive Bader analysis application could be developed, which enables interactive visual inspection of the 3D structures of crystals.

In the field of solar-cell design, advanced molecular-rendering techniques enable solar-cell designers and molecular-dynamics researchers to better understand their simulation data. Another central domain area for the visualisation community is medical visualisation. Consequently, new interdisciplinary results could also be achieved, whereby focus lies on large-data analysis and pattern extraction. One example is the novel use of visualisation for the quantitative analysis of knee-movement patterns in time-varying data sets. Furthermore, a visualisation framework for the analysis of blood-flow characteristics based on image acquisition of velocity data for beating hearts (4D MRI) has been developed.

Apart from the intercommunity efforts

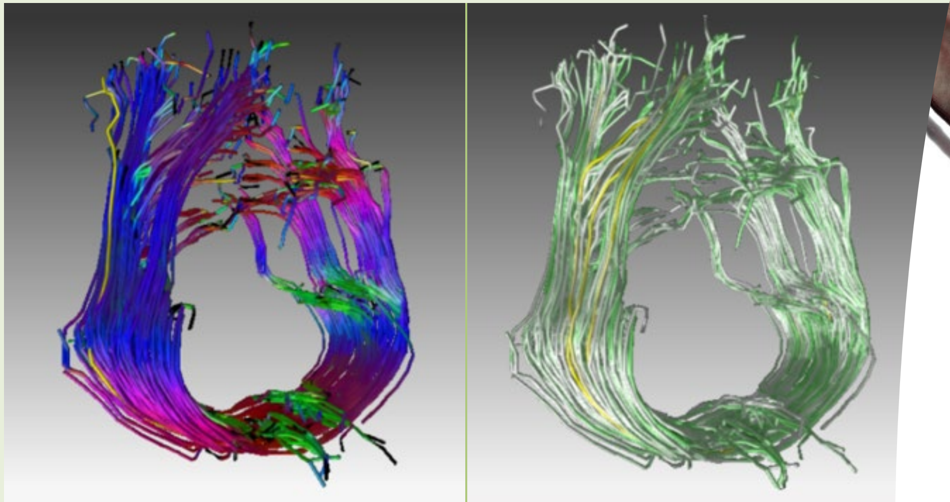


Figure 7. Diffusion-tensor imaging (DTI) in combination with fibre-tracking algorithms enables visualisation and characterisation of white-matter structures in the brain. Low spatial resolution and low signal-to-noise ratio of DTI has raised concerns regarding the reliability of the obtained fibre bundles. Combining deterministic and stochastic approaches leads to more reliable results. The images show a visualisation of DTI fibres using streamtubes with colours mapped to the normal vector direction (left) and mapping uncertainty to the saturation of the colour (right).

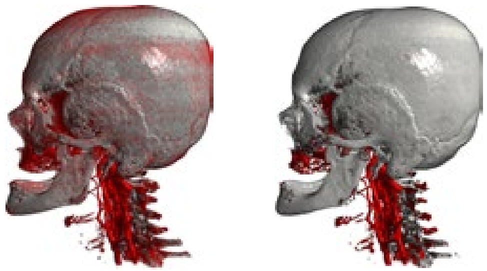


Figure 8. By respecting boundaries in the reconstruction of sampled data, artefacts can be avoided such as the redness of the white-bone structures in the left image.

Main position in our three-pillar model (see page 5)

Figure 9. Illumination of volumetric data using photon mapping. The method only recomputes photons that are affected by changes of parameters enabling interactive exploration of the data during parameter changes.

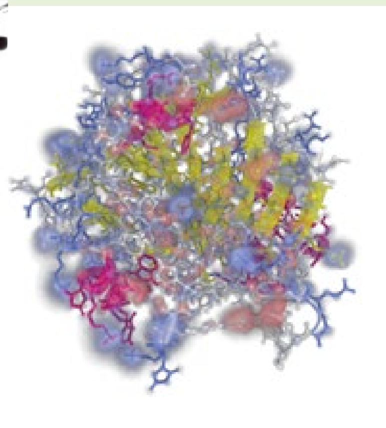


Figure 10. Visualisation of a protein combining hybrid data from different sources using a hybrid visualisation of geometric protein representations and volumetric data. Our improved A-buffer algorithm is capable of rendering the entire scene with a performance increase of 5.9 times compared to prevalent techniques.

and applied visualisation work, the visualisation community has made high-impact contributions to the foundations of volume rendering in areas such as:

- *Uncertainty visualisation, verification, and error reduction:* In the context of fibre tracking in the brain, fundamental aspects of uncertainty have been studied and interactive guidance paradigms have been applied (see figure 7).
- *Improving visualisation of boundaries:* Fundamental work on volume rendering has resulted in novel ways to deal with tissue boundaries in medical volume data using knowledge based regression of reconstruction kernels (see figure 8).
- *Volumetric Illumination:* Progressive development of shading algorithms resulting in interactive rendering of multiple scattering events using photon-mapping techniques. (see figure 9).
- *Depth complexity in mixed-mode rendering:* Development of heuristics that minimise memory footprint on the GPU depth sorting geometry mixed with volume data. (see figure 10).

Besides these research results, researchers in the visualisation community have been involved in the development of the Inviwo open-source visualisation framework. This framework builds the basis for most ongoing projects within SeRC and maximises the synergy between the individual visualisation projects. Furthermore, new industry collaborations have been established. Within this process, the research output of the visualisation community was instrumental.

Read more on
www.e-science.se/visualisation

SUCCESS STORY:
ELECTRONIC STRUCTURE

Materials science is currently enjoying a golden age, due to the increase in understanding of the underlying atomic phenomena. Studying materials at high pressure is of relevance for everything from coatings of industrial tools to the very fabric of Earth's inner core. If we understand how matter works at high pressure, we will be in a better position to develop materials that withstand extreme conditions.

In collaboration with experimentalists, researchers in the applied community *Electronic Structure* recently discovered a new phenomenon in the metal osmium when subjected to ultrahigh pressure. Osmium is the most dense of all elements, with its hardness rivalling that of diamond. It is being used in fountain pen nibs, electrical contacts and other applications where extreme hardness is required. While subjecting an osmium sample to the record-high pressure of four million atmospheres, measurements indicated an anomaly in the relation between the interatomic distances.

In order to understand its origin, SeRC theoreticians performed highly precise simulations of the electronic structure – an effort which required millions of core-hours to reach the required precision. Astonishingly, the anomaly could not be attributed to any reconfiguration of the valence electrons (see figure 11). Instead, it was found that even the innermost electrons begin to interact with each other, a phenomenon never witnessed before.

The phenomenon means that we can start searching for brand new states of matter. It opens up a whole box of new questions for future research, and the research results were published in the highly ranked journal *Nature*.

New simulation tools are currently being developed. The SeRC environment allows material scientists to coordinate their needs with the core communities, and take advantage of large-scale parallel resources. Such coordinated efforts will be essential to study technologically relevant materials at extreme conditions.

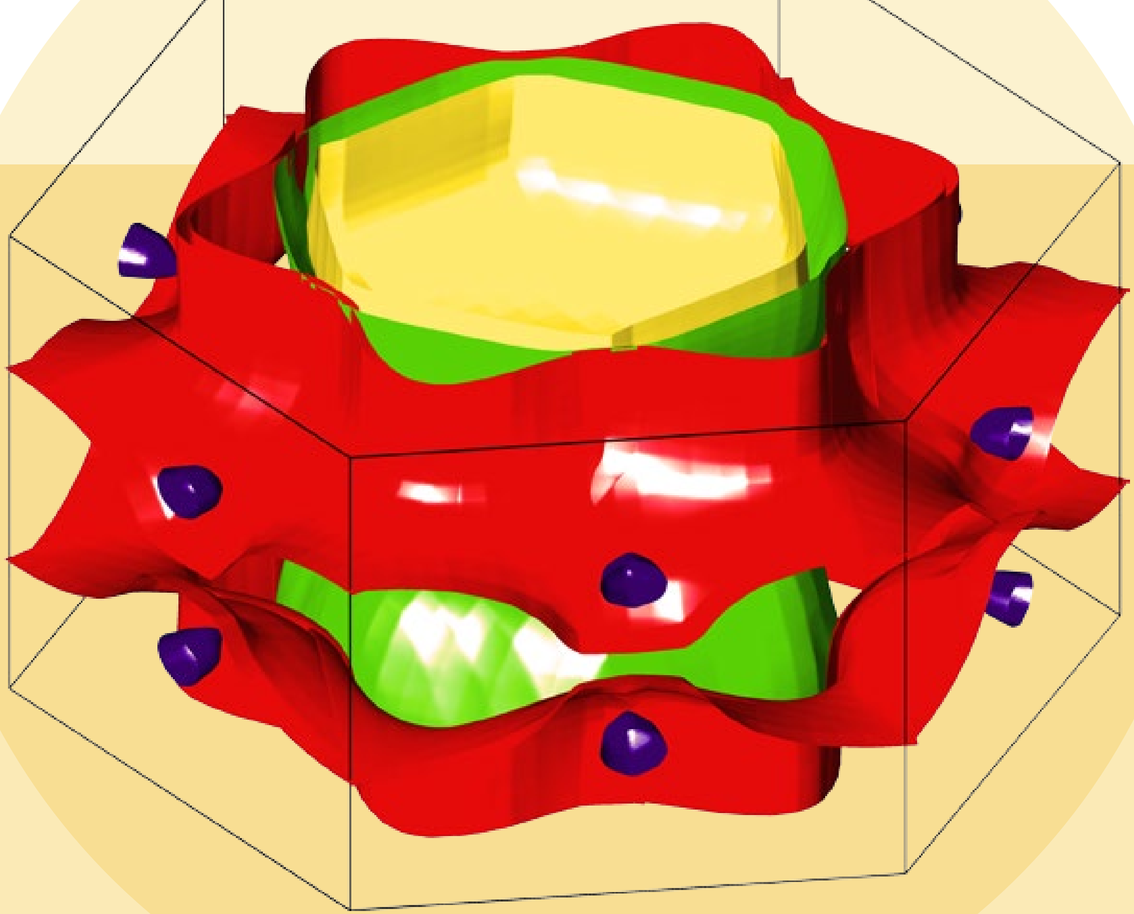


Figure 11. Valence electron constant energy surface (Fermi surface) of osmium. Properties of metals can be related to the valence electrons, which are responsible for bonding. However, accurate calculations show that the structural anomaly at high pressure could not be attributed to any qualitative reconfiguration of the valence electrons. (Picture courtesy of Q. Feng)

Read more on
www.e-science.se/electronic-structure

Main position in our three-pillar model (see page 5)

3. The future

What we have seen up to now is only the beginning. e-Science is here to stay, and the SeRC concept constitutes the perfect greenhouse.

e-SCIENCE AGENDA

In its first five years, SeRC has had a tremendous success in establishing e-Science in Sweden and fostering the e-Science paradigm in many research areas. e-Science is now well established and a priority area at the SeRC partner universities.

The next phase of SeRC (2015–2019) will on the one hand further consolidate these efforts working towards a long-lasting e-Science environment, and on the other hand increase activities on emerging technologies, such as the already initiated exascale or big-data technologies.

> SeRC has had a tremendous success in establishing e-Science in Sweden."

An important document in shaping the future of e-Science in Sweden is the recent report from Vetenskapsrådet *Swedish Science Case for e-Infrastructure* (**www.e-science.se/sscei**). This document discusses strategic e-Science development in Sweden and makes a number of recommendations that will help guide future SeRC developments. Key findings from a SeRC perspective include:

- Development of methods, tools, and software within core disciplines is necessary to make breakthroughs.
- Advanced and long-term user support and human infrastructures are keys to e-Science adoption.
- The simulation paradigm dominates the current Swedish needs for e-infrastructure. A complementary and more data-centric aspect of e-Science should be promoted.
- e-Social science and e-humanities are potentially very large users, but need active support like other communities new to e-Science.
- e-Science methods and tools are in increasing demand and will be instrumental in increasing interaction between tool makers and tool users.

Enacting these recommendations entails work at several levels ranging from infrastructure and tool development to policy definitions. In its strategy process, SeRC has defined an agenda for the next five years. This agenda addresses many of the items from the report and describes how SeRC is in a unique position to spearhead this work.

Below, we give an overview of these new SeRC initiatives defined to evolve SeRC as

an organisation as well as paving the path for the next stage of e-Science development and deployment in Sweden.

IMPACT

The impact of e-Science can be found in all areas of academia. The use of basic e-Science in new domains can generate fundamentally new and important results. At the same time, access to advanced e-Science tools and infrastructure enables the leading research groups that are spear-heading Swedish e-Science to compete at the international forefront.

In view of this, SeRC intends to intensify collaborations with relevant Swedish groups and universities currently not part of SeRC and aims for a national scope in domains like bioinformatics, numerical analysis and material science. By expanding such collaborations, SeRC will develop into a truly national organisation. This will also allow SeRC to take responsibility to further develop the Swedish e-infrastructure landscape together with SNIC.

The impact of broad adoption of e-Science methodology cannot be overestimated. Through extensive collaborations with industry and governmental agencies SeRC generates direct impact in society and contributes to societal development and commercial competitiveness. SeRC has several industrial representatives on its advisory board, and we are delighted with their interest and engagement in learning how computing can change what they do, for instance at our annual meetings. One of the primary indirect impact mechanisms for SeRC is knowledge transfer in the form of examined PhDs, who hold unique experiences of e-Science and form a network consisting of the next generation of e-scientists.

The single largest overall successes of SeRC is that it has helped application researchers and computational experts to find each other and speak with one voice. Large-scale data analysis and simulation have been introduced in areas where it has not been used before, the strongest computational groups in the country collaborate internationally instead of competing nationally, and we will keep redefining these boundaries by identifying areas where the combination of computational and application research excellence make a field ripe for disruptive changes to the science.

INITIATIVE: MULTIDISCIPLINARY COLLABORATION PROGRAMMES

In the first phase of SeRC, larger, multidisciplinary constellations have been prototyped through a *multidisciplinary collaboration programme* (MCP) promoting multidisciplinary approaches to strategic areas with high potential gain. With *eCPC* (see page 11) as SeRC's first MCP flagship, followed by *Visualisation In e-Science Applications* (see pages 14–15) and *SESSI* (SeRC Exascale Simulation Software Initiative), we will now build on these successes and further develop the MCPs by consolidating the SeRC efforts into larger constellations.

A key requirement of MCPs is the existence of external third-party support contributing to the programme goals. These multiple funding streams are one component to ensure the sustainability of SeRC efforts. For 2015–2019, three additional MCPs have been started: *Data-Driven Computational Materials Design, FAST Climate Science* and *Brain-IT.*

INITIATIVE: SCIENTIFIC COMPUTING LAB

SeRC groups are engaged in computational method and infrastructure development, a necessary ingredient for world-class computer-based science. With architectural changes, driven partly by the challenge to build exascale systems, these efforts need to be re-enforced and strengthened. Developments such as massively increased core-counts, large vector units, deep memory hierarchies, and similar advances require significant efforts in the development of efficient, scalable methods and implementations.

Such work is planned in the multidisciplinary collaboration programs referred to earlier. These constitute ideal cases for the SeRC vision of integrating researchers in the three pillars described earlier, with collaboration between application areas, e-infrastructure and methods researchers being facilitated by the e-Science experts in the "human e-cloud".

Following international examples, for instance from NCSA at UIUC, we will prototype a scientific computing lab, where researchers from applications, methods, and infrastructure can collaborate efficiently in such an environment. A physical interaction space created close to PDC is a key component in this endeavour. With this lab, SeRC will build the nucleus of the "human e-cloud" identified as a key ingredient above.

INITIATIVE: DATA-DRIVEN SCIENCE

The data deluge that arises from new scientific instruments, large simulations, and data on the internet together with new technologies of how to handle and analyse these data has significant impact on e-Science methodology. SeRC is therefore embracing big data, with an initial emphasis on life science. This includes research regarding storage, management, integration, visualisation, and analysis of big data.

In recent years, new platforms and tools have appeared that can efficiently and cost-effectively store and process up to petabytes of data. This allows many organisations to handle data that previously was considered too expensive to store and manage. This data-driven science trend is transforming scientific research, by enabling data-driven discovery and prediction. The skills required for data analytics at large scale include data management on public and private clouds, data-parallel algorithms, and proficiency with a complex ecosystem of tools and platforms such as Hadoop. These skills are currently not widely available within the existing communities; one of the goals for SeRC is to help transfer knowledge on the use of methods and tools from data science to enable new research methodologies in other SeRC communities.

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